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Sufficient condition for stability of *N*-body system with attractive pair potentials

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Abstract

The system of N particles that are non-fermions interacting with non-positive pair potentials is considered. Each system is represented by a graph with points for particles and links for existence of bound states in the corresponding particle pair. A general sufficient condition for stability (the stability is defined as the existence of a bound state with the energy below all dissociation thresholds) is formulated as a theorem: any connected graph represents a stable system. The theorem also shows that the system may dissociate only into those clusters that contain full connected components of the graph. The applications to stability of nuclei are discussed.

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1. Introduction

In quantum mechanics it is very important to understand whether the system stays as a whole or dissociates into a number of subsystems. This question of stability is crucial for various issues in nuclear, atomic and molecular physics. The spectrum of a physical system always has a zero energy threshold corresponding to independent scattering of all particles. Other continuum (dissociation) thresholds correspond to all possible ways to decompose all particles into clusters, which are either bound subsystems or single particles. For a given decomposition the sum of a cluster's ground-state energies (zero if a cluster consists of one particle) is the energy of the continuum threshold. Below all continuum thresholds in the spectrum there lie only isolated eigenvalues corresponding to the bound states of the whole system [1].

From the spectral point of view, and this is how we shall understand this, stability is the presence of a bound state below any continuum in the spectrum. For the system this would mean that dissociation is unfavourable for gaining the lowest energy. In contrast, the system of N particles is unstable if the lowest energy $E_1 + E_2 + \cdots + E_n$ is attained as a sum of ground-state energies of n bound clusters (the energy E_i is zero if the cluster i consists of one particle).



Figure 1. All different types of graphs for three-body systems, links between particles symbolize the existence of a bound state in a pair.

The factors that affect stability of quantum systems may be classified by three causes of instability [3]: (i) kinetic motion; (ii) the Pauli principle; (iii) repulsive forces. The absence of parallels with classical mechanics makes the first two reasons the most intriguing. In actual atomic and molecular systems these factors appear mixed and sometimes it is practical to distil the prevailing factor. For general understanding, as well, it is useful to consider systems where only one of the reasons predicates the instability. Here we shall deal with kinetic instability.

The question of stability for particles with attractive pair-interactions, i.e. $V_{ik} \leq 0$, is nontrivial. It is well known that the attractive potential in three dimensions must have a minimal strength to bind a particle. As a consequence, the Hamiltonian with weak, yet attractive, pair interactions may have only positive energy, which means total instability for the system [1, 3]. For physical reasons weak pair interactions are unable to confine kinetic motion and the system falls apart becoming kinetically unstable.

Interesting natural phenomena, where kinetic instability plays a decisive role are associated with exotic nuclei on the edge of stable nuclear chart, especially Borromean nuclei [5]. These are loosely bound systems such as nuclei ⁶He and ¹¹Li, which have a pronounced three-body structure with no subsystems bound. In particular, the nucleus ⁶He comprises an α -particle and two neutrons, which together are bound in spite of no bound states in pairs such as α -particle and neutron or two neutrons. Italian heraldry prompted the term Borromean implying three interlaced rings on the Borromean coat of arms, where removing one ring dismantles all three. In some models the pair interactions in the three-body system ⁶He are attractive which raises the question of what is the sufficient strength of attractive pair interactions that makes ⁶He system stable. In [2, 3] one can find necessary conditions for stability of such systems. Here we shall derive a simple sufficient condition for stability.

2. Graph representation

Throughout the paper we shall deal with particles that are non-fermions, thus switching off the Pauli principle. In a system of N particles the situation can be depicted with a graph. Scatter N particles as points on a plane and connect two points (*i*) and (*k*) with a link if the pair (*ik*) has a bound state. Figure 1 shows all possibilities for three particles. In [3, 4] simple necessary conditions for binding are expressed through fractions of binding and mass ratios. From these conditions it follows that the system in figure 1(*a*) is definitely unbound if fractions of binding are very small, but can be bound otherwise. The stable system with a graph in figure 1(*a*) is called Borromean, as we call all systems with no bound subsystems. If interactions in figure 1(*b*) are loose, particle 3 will never couple to the bound pair (12). Systems in figures 1(*c*), (*d*) have a good chance of being stable. In fact, the links in these graphs play the role of 'threads' between the particles, and if no particle or group of particles can be taken out without cutting a 'thread' the system is stable. The following theorem holds.



Figure 2. Choice of coordinates for two clusters. Circles marked with a cross refer to the centres of gravity for each cluster.

Theorem 1. For a system of particles that are non-fermions and interact through negative pair potentials any connected graph represents a stable system.

Proof. There could be a number of bosons in the system. However, the ground-state wavefunction for the bound state will not change if we treat bosons as distinguishable particles because this function is non-negative and non-degenerate [1] and thus all such functions automatically possess required symmetry. Thus from now on we treat all particles as distinguishable. We shall also assume that pair interactions conserve the parity. We have to prove that the system as a whole has the energy less than any of its rearrangements into bound clusters.

First, let us assume that there are two bound clusters with particle (a) in the first cluster, and particle (b) in the second cluster, so that the pair (ab) has a bound state with some energy e_{ab} . We shall call such clusters connected. Let particles (a) and (b) label the corresponding clusters. We shall show that if both clusters have bound states with energies E_a and E_b , the energy of two connected clusters united in one system is less than $E_a + E_b$. The particles in the first cluster are (a, 1, 2, ..., k), while the second cluster consists of (b, k + 1, ..., l). Let $(\mathbf{r}_a, \mathbf{r}_b, \mathbf{r}_i)$ (i = 1, ..., l) denote the vector positions of particles, then relative coordinates are chosen as $\mathbf{x}_i = \mathbf{r}_i - \mathbf{r}_a$ (i = 1, ..., k) for the first cluster and $\mathbf{x}_i = \mathbf{r}_i - \mathbf{r}_b$ (i = k + 1, ..., l)for the second cluster. Figure 2 illustrates the choice of relative coordinates in clusters. R denotes the relative coordinate between centres of mass in both clusters (see figure 2), and $M_a = m_a + m_1 + \cdots + m_k$ and $M_b = m_b + m_{k+1} + \cdots + m_l$ denote total masses of the first and the second cluster. With the help of the variational principle we shall seek the lower bound for the total energy. Because all interactions between clusters are non-positive we can put them to zero, all except V_{ab} , and this would only increase the energy of the whole system. Then the Hamiltonian of the relative motion in two clusters together with the centre of mass motion separated takes the form

$$H = H_a(\mathbf{x}) + H_b(\mathbf{x}) - \frac{M_a + M_b}{2M_a M_b} \Delta_R + V_{ab}.$$
 (1)

Here $H_a(\mathbf{x})$ and $H_b(\mathbf{x})$ are the Hamiltonians of relative motion in each cluster (we use units where $\hbar = 1$). In coordinates \mathbf{x}_i they have the form [6]

$$H_a(\mathbf{x}) = -\sum_{i=1}^k \frac{1}{2\mu_{ai}} \Delta_i - \frac{1}{m_a} \sum_{1 \le i < j \le k} \nabla_i \cdot \nabla_j + U_a(\mathbf{x})$$
(2)

$$H_b(\mathbf{x}) = -\sum_{i=k+1}^l \frac{1}{2\mu_{bi}} \Delta_i - \frac{1}{m_b} \sum_{k+1 \leqslant i < j \leqslant l} \nabla_i \cdot \nabla_j + U_b(\mathbf{x})$$
(3)

where $\mu_{ai} = m_a m_i / (m_a + m_i)$, $\mu_{bi} = m_b m_i / (m_b + m_i)$ and U_a , U_b denote sums of pair interactions in corresponding clusters. The label *i* below the differential operator means partial differentiation with respect to coordinate \mathbf{x}_i . The last term in equation (1) is responsible for the relative motion of clusters with respect to their centres of mass.

Now let us change the variables and instead of the set {**x**, **R**} use coordinates { $\tilde{\mathbf{x}}$, \mathbf{r}_{ab} }, where $\tilde{\mathbf{x}}_i = \mathbf{x}_i$ and $\mathbf{r}_{ab} = \mathbf{r}_b - \mathbf{r}_a$ (see figure 2)

$$\mathbf{r}_{ab} = \mathbf{R} + \frac{1}{M_a} \sum_{i=1}^k m_i \mathbf{x}_i - \frac{1}{M_b} \sum_{i=k+1}^l m_i \mathbf{x}_i.$$
(4)

Using equation (4) we find that the differential operators transform as follows:

$$\nabla_i = \tilde{\nabla}_i + \frac{m_i}{M_a} \nabla_{ab} \qquad (1 \leqslant i \leqslant k) \tag{5}$$

$$\nabla_i = \tilde{\nabla}_i - \frac{m_i}{M_b} \nabla_{ab} \qquad (k+1 \leqslant i \leqslant l) \tag{6}$$

$$\nabla_R = \nabla_{ab}.\tag{7}$$

Here $\bar{\nabla}_i$ and ∇_{ab} mean differentiation with respect to $\tilde{\mathbf{x}}_i$ and \mathbf{r}_{ab} . We have to rewrite in new coordinates (1). When we substitute expressions (5)–(7) into equation (1) we shall get the same equation in new variables $\tilde{\mathbf{x}}_i$ plus mixed terms such as $\bar{\nabla}_i \cdot \nabla_{ab}$ and the term with Δ_{ab} . Let us find the expression for the coefficient in front of Δ_{ab} . Collecting all terms in front of it gives

$$\sum_{i=1}^{k} \left(\frac{1}{2m_a} - \frac{1}{2\mu_{ai}} \right) \frac{m_i^2}{M_a^2} + \sum_{i=k+1}^{l} \left(\frac{1}{2m_b} - \frac{1}{2\mu_{bi}} \right) \frac{m_i^2}{M_b^2} - \frac{1}{2m_a} \frac{(M_a - m_a)^2}{M_a^2} - \frac{1}{2m_b} \frac{(M_b - m_b)^2}{M_b^2} - \frac{M_a + M_b}{2M_a M_b} = -\frac{1}{2\mu_{ab}}$$
(8)

where $\mu_{ab} = m_a m_b / (m_a + m_b)$. Thus we rewrite the Hamiltonian in new coordinates

$$H = H_a(\tilde{\mathbf{x}}) + H_b(\tilde{\mathbf{x}}) + \left(-\frac{1}{2\mu_{ab}}\Delta_{ab} + V_{ab}\right) + \sum_{i=1}^l C_i \tilde{\nabla}_i \cdot \nabla_{ab}$$
(9)

where C_i are some coefficients depending on masses.

Because the clusters are bound we have $H_a \Psi_a(\tilde{\mathbf{x}}) = E_a \Psi_a(\tilde{\mathbf{x}})$ and $H_b \Psi_b(\tilde{\mathbf{x}}) = E_b \Psi_b(\tilde{\mathbf{x}})$. Taking the ground-state wavefunction $\phi_{ab}(\mathbf{r}_{ab})$ of the bound pair (*ab*) construct the trial function $\chi(\tilde{\mathbf{x}}, \mathbf{r}_{ab}) = \Psi_a \Psi_b \phi_{ab}$, where each function in the product is normalized.

The wavefunction ϕ_{ab} has determined parity $\phi_{ab}(\mathbf{r}_{ab}) = \pm \phi_{ab}(-\mathbf{r}_{ab})$. Passing from \mathbf{r}_{ab} to $-\mathbf{r}_{ab}$ in the variables of integration we shall prove that $\langle \chi | \tilde{\nabla}_i \cdot \nabla_{ab} | \chi \rangle = 0$. Thus substituting the trial function into $\langle \chi | H | \chi \rangle$ will cancel the contribution from the last term in equation (9) and yield the energy $E_a + E_b + e_{ab}$. By the variational principle the energy of *H* is less than $E_a + E_b$ at least by e_{ab} and this proves the preliminary statement. (Note that the variational argument does not show that two clusters are bound when together, it only shows that $E_a + E_b$ is not the lowest possible energy.)

Assume by contradiction that the system of N particles with connected graph is unstable and the lowest energy $E_1 + E_2 + \cdots + E_n$ is attained as a sum of ground-state energies of n bound clusters. There should exist particle (a) in the first cluster, which forms a bound state with particle (b) in some cluster (i), otherwise all particles in cluster (1) would be disconnected from all other particles in contradiction with condition of the theorem. But in this case $E_1 + \cdots + E_n$ is not the lowest energy, because we proved that clusters (1) and (i) taken together have the energy lower than $E_1 + E_i$. The obtained contradiction proves the theorem.

As discussed previously the question of stability for a system with attractive pair potentials is far from trivial. In arbitrary system with attractive pair potentials each subsystem has a good chance of being bound and any study of stability would involve *accurate* measuring of the energy for all subsystems. Only after that using the variational principle one might show that the total energy is lower than any dissociation threshold. From simple combinatorics that would require accurate few-body calculation of the energy for $(2^N - N - 2)$ subsystems which is hopeless (for example, for six particles this makes 56 subsystems). From this viewpoint the proved theorem is a useful tool for testing stability, because it requires checking the existence of bound states only in pairs of particles which is simpler than to determine exactly the energy of the ground state. The following corollary immediately follows from the proof.

Corollary 1. A system of particles which are non-fermions with $V_{ik} \leq 0$ in one and two dimensions is always stable. For a system of bosons with $V_{ik} \leq 0$ in three dimensions stability follows from the existence of a bound state in a pair of bosons.

It is well known that in one and two dimensions a pair of particles with $V_{ik} \leq 0$ has a bound state, so the graph for the whole system becomes fully connected in all cases mentioned in the corollary. The theorem does not work for fermions. To see this take for example a three-body system with two particles of equal mass 1 and 2, which try to bind to the core having the infinite mass 3, so that $V_{12} = 0$ and $V_{13}(\mathbf{r}) = V_{23}(\mathbf{r}) = U(\mathbf{r})$. If potential $U(\mathbf{r})$ supports only one bound state then there would be only one bound state in the three-body system, which is symmetric with respect to the interchange of particles 1 and 2. If particles 1 and 2 are fermions the whole system is unstable because there are no bound states with required symmetry, nevertheless the graph for the system is obviously connected.

Each graph has a number of connected components (if there is only one component the system is stable). The following useful corollary substantially reduces the possible ways of dissociation of a system.

Corollary 2. If the system dissociates with the lowest possible energy, it may dissociate only into clusters that contain fully connected components.

This immediately follows from the proof of the theorem. Let the lowest energy $E_1 + E_2 + \cdots + E_n$ be attained as a sum of ground-state energies of *n* bound clusters. From the proof it follows that each particle in cluster (1) is disconnected from particles in other clusters and this means that it contains full connected components of the graph.

In the next theorem we prove the lower bound for the energy that is useful for further restrictions of possible types of dissociation.

Theorem 2. Let n clusters consisting of particles that are non-fermions and interact through negative pair potentials have the energies E_1, \ldots, E_n . Additionally assume that in each cluster (i) there exists a particle c_i ($i = 1, \ldots, n$), so that n particles c_i have a bound state with the energy $e(c_1, \ldots, c_n)$. Then the total energy of n clusters together is less than $E_1 + \cdots + E_n + e(c_1, \ldots, c_n)$.

Proof. The proof follows the same lines as that of theorem 1. The clusters from 1 to *n* contain the particles $\{c_1, 1, 2, ..., k_1\}, \{c_2, k_1 + 1, ..., k_2\}, ..., \{c_n, k_{n-1} + 1, ..., k_n\}$. Let m_i , \mathbf{r}_i $(i = 1, ..., k_n)$ and m_{c_j} , \mathbf{r}_{c_j} (j = 1, ..., n) denote the vector positions and masses of all particles. As before to separate the centre of mass motion from each cluster we choose



Figure 3. Choice of coordinates for *n* clusters in the proof of theorem 2.

relative coordinates in each cluster $\mathbf{x}_s = \mathbf{r}_s - \mathbf{r}_{c_j}$, where $k_{j-1} + 1 \leq s \leq k_j$ and j = 1, 2, ..., n (see figure 3). The relative motion of clusters is described by translation-invariant coordinates of clusters' centres of mass

$$\mathbf{R}_{j} = \frac{1}{M_{c_{j}}} \left(m_{c_{j}} \mathbf{r}_{c_{j}} + \sum_{s=k_{j-1}+1}^{k_{j}} m_{s} \mathbf{r}_{s} \right) - \frac{1}{M_{c_{n}}} \left(m_{c_{n}} \mathbf{r}_{c_{n}} + \sum_{s=k_{n-1}+1}^{k_{n}} m_{s} \mathbf{r}_{s} \right)$$
(10)

where j = 1, 2, ..., n - 1 and $M_{c_j} = m_{c_j} + \sum_{s=k_{j-1}+1}^{k_j} m_s$ is the mass of the cluster containing the particle c_j . The particles c_i (i = 1, ..., n) form a bound system. In this system we choose relative coordinates as $\mathbf{f}_j = \mathbf{r}_{c_j} - \mathbf{r}_{c_n}$ (j = 1, ..., n - 1) (see figure 3). The Hamiltonian of this system with separated centre of mass motion

$$h(\mathbf{f}) = -\sum_{i=1}^{n-1} \frac{1}{2\mu_{c_i c_n}} \Delta_{f_i} - \frac{1}{m_{c_n}} \sum_{i< j=1}^{n-1} \nabla_{f_i} \cdot \nabla_{f_j} + U(\mathbf{f})$$
(11)

where $\mu_{c_i c_n}$ is the reduced mass for particles c_i and c_n and $U(\mathbf{f})$ is the sum of interactions between particles c_i . By condition of the theorem there is a bound state wavefunction $\Phi(\mathbf{f})$ depending on relative coordinates \mathbf{f}_i so that $h(\mathbf{f})\Phi(\mathbf{f}) = e(c_1, \dots, c_n)\Phi(\mathbf{f})$.

Because we seek an upper bound for the energy and all potentials are non-positive we can put all pair interactions between clusters to zero except the term $U(\mathbf{f})$. The Hamiltonian of the whole system takes the form

$$H = \sum_{j=1}^{n} H_{c_j}(\mathbf{x}) + T_R + U(\mathbf{f}).$$
 (12)

Here the Hamiltonian of relative motion in each cluster

$$H_{c_j}(\mathbf{x}) = -\sum_{s=k_{j-1}+1}^{k_j} \frac{1}{2\mu_{sc_j}} \Delta_s - \frac{1}{m_{c_j}} \sum_{s< p=k_{j-1}+1}^{k_j} \nabla_s \cdot \nabla_p + U_{c_j}(\mathbf{x})$$
(13)

where $U_{c_j}(\mathbf{x})$ is the sum of pair interactions in the cluster with the particle c_j . The second term in equation (12) is the kinetic energy of clusters' relative motion with respect to the clusters' centres of mass

$$T_R = -\sum_{j=1}^{n-1} \frac{M_{c_j} + M_{c_n}}{2M_{c_j}M_{c_n}} \Delta_{R_j} - \frac{1}{M_{c_n}} \sum_{i< j=1}^{n-1} \nabla_{R_i} \cdot \nabla_{R_j}.$$
 (14)

Now let us pass from the set of variables $\{\mathbf{x}, \mathbf{R}\}$ to the set $\{\tilde{\mathbf{x}}, \mathbf{f}\}$, where $\tilde{\mathbf{x}}_i = \mathbf{x}_i$. Just as in equation (4) we get

$$\mathbf{f}_{j} = \mathbf{R}_{j} + \frac{1}{M_{c_{n}}} \sum_{i=k_{n-1}+1}^{k_{n}} m_{i} \mathbf{x}_{i} - \frac{1}{M_{c_{j}}} \sum_{i=k_{j-1}+1}^{k_{j}} m_{i} \mathbf{x}_{i}.$$
(15)

Using equation (15) we find that the differential operators transform as follows:

$$\nabla_i = \tilde{\nabla}_i - \frac{m_i}{M_{c_j}} \nabla_{f_j} \quad (k_{j-1} + 1 \leqslant i \leqslant k_j) \ (j \leqslant n-1) \tag{16}$$

$$\nabla_i = \tilde{\nabla}_i + \frac{m_i}{M_{c_n}} \sum_{j=1}^{n-1} \nabla_{f_j} \quad (k_{n-1} + 1 \leqslant i \leqslant k_n)$$

$$\tag{17}$$

$$\nabla_{R_j} = \nabla_{f_j}.\tag{18}$$

Just like in the proof of theorem 1, when we substitute equations (16)–(18) into expression for the Hamiltonian equation (12) terms appear of the type $-\Delta_{f_j}$, $\nabla_{f_i} \cdot \nabla_{f_j}$ and mixed terms such as $\tilde{\nabla}_i \cdot \nabla_{f_j}$. The coefficient in front of $-\Delta_{f_j}$ has the expression

$$\frac{M_{c_j} + M_{c_n}}{2M_{c_j}M_{c_n}} + \sum_{s=k_{j-1}+1}^{k_j} \frac{m_s + m_{c_j}}{2m_s m_{c_j}} \left(\frac{m_s}{M_{c_j}}\right)^2 + \frac{1}{m_{c_j}M_{c_j}^2} \sum_{s< p=k_{j-1}+1}^{k_j} m_s m_p \tag{19}$$

$$+\sum_{s=k_{n-1}+1}^{k_n} \frac{m_s + m_{c_n}}{2m_s m_{c_n}} \left(\frac{m_s}{M_{c_n}}\right)^2 + \frac{1}{m_{c_n} M_{c_n}^2} \sum_{s< p=k_{n-1}+1}^{k_n} m_s m_p = \frac{1}{2\mu_{c_j c_n}}.$$
 (20)

The coefficient in front of $-\nabla_{f_i} \cdot \nabla_{f_i}$ has the expression

$$\frac{1}{M_{c_n}} + \frac{1}{m_{c_n}M_{c_n}^2} \sum_{s=k_{n-1}+1}^{k_n} \left(m_s + m_{c_n}\right)m_s + \frac{2}{m_{c_n}M_{c_n}^2} \sum_{s< p=k_{n-1}+1}^{k_n} m_s m_p = \frac{1}{m_{c_n}}.$$
(21)

Finally we obtain

$$H = \sum_{j=1}^{n} H_{c_j}(\tilde{\mathbf{x}}) + h(\mathbf{f}) + \sum_{i,j} C_{ij} \tilde{\nabla}_i \cdot \nabla_{f_j}.$$
(22)

Let $\Psi_j(\tilde{\mathbf{x}})$ be the normalized ground-state wavefunction corresponding to the energy E_j of the cluster Hamiltonian H_{c_j} . To get the upper bound for the energy we construct the trial function

$$\chi(\tilde{\mathbf{x}}, \mathbf{f}) = \Phi(\mathbf{f}) \prod_{j=1}^{n} \Psi_j(\tilde{\mathbf{x}}).$$
(23)

The function $\Phi(\mathbf{f})$ has determined parity with respect to transformation $\mathbf{f}_j \rightarrow -\mathbf{f}_j$ for all j = 1, ..., n - 1 and this cancels all mixed terms in equation (22). The trial function in equation (23) gives the energy $E_1 + \cdots + E_n + e(c_1, ..., c_n)$ and this proves the theorem. \Box

Let us assume, for example, that the graph for the system has three connected components represented by three subsystems A, B, C. Suppose there are three particles, one in each cluster, which form a stable system (this would be a Borromean system, because clusters A, B, C are not connected). Then according to theorem 2 the whole system may dissociate only in two parts such as AB and C, because decaying into three parts does not correspond to the lowest possible energy.

Another example applies to the system of N bosons interacting with attractive potentials. Physically, the effective mass in the system increases with the number of bosons and this makes the system more stable. It would be right to expect that if this system becomes stable for $N = N_0$ then it would be stable for $N \ge N_0$. However, such intuitive conjectures are hard to prove, incidentally, it is still an open problem to prove that adding one electron to unstable negative ion does not make it stable [7]. Theorem 2 says that if the system of bosons is unstable for $N < N_0$ and stable for $N = N_0$ then there would be infinitely many $N > N_0$ for which the system would be stable and the difference between two consecutive numbers corresponding to stable systems is less than or equal to $N_0 - 1$.

3. Conclusions

We have derived a general result that gives sufficient condition for stability and restricts possible dissociations. This approach can find application in nuclear physics for analysis of loosely bound nuclei at the border of the stable nuclear chart. The problem there is often simplified, treating clusters as separate structureless particles such as α -particle (this is a successful approach to many nuclei). The interaction between those clusters is often modelled as attractive which leaves only one destructive factor—kinetic instability. For these systems the approach can find its applications. Not only does theorem 1 give a sufficient condition, it can help to construct efficient necessary conditions for binding (or sufficient conditions for instability). When it comes to necessary conditions these graphs show where to concentrate the effort. In formulating necessary conditions one simply follows the old saying: the chain is no stronger than its weakest link.

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