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Monotonicity of energy eigenvalues for Coulomb systems

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Abstract. Generalising results by Reed/Simon and Thirring, we prove for a large class of Hamiltonians (among others, Hamiltonians of Coulomb systems) which can be written in the form $H(\alpha)=H_0+\alpha H'$ that their eigenvalues decrease with increasing α. We apply this result to Coulomb systems in which the distances between the infinitely heavy particles are varying and also use it to obtain a completion and simplification of Adamowski *et al*'s proof for the stability of the biexciton.

1. Introduction

In comparison with the vast number of calculations of energies in Coulomb systems, there are only a few rigorous statements concerning the qualitative behaviour of the energy as a function of some parameter α. Such results help to judge the accuracy of approximate energy calculations. The most famous example of such qualitative statements is that the first eigenvalue, $E_1(\alpha)$, of the Hamiltonian $H(\alpha)=H_0+\alpha H'$ is a concave function of α. From the concavity we conclude the monotonicity of the ground-state energy (lemma 4). In order to get analogous results for the excited-state energies $E_i(\alpha)$, $i>1$, we present in lemma 5 a strong generalisation of a proposition by Reed and Simon (1978). Thus we can prove for $\alpha\geqslant 0$ that $E_i(\alpha)\leqslant 0$ and $E_i(\alpha)/\alpha$ is decreasing if $H_0=\Sigma-\Delta_i/m_i$ and $H'=\Sigma\, V_i(\boldsymbol{r}_i)+\Sigma\, V_{ij}(\boldsymbol{r}_i,\boldsymbol{r}_j)$ with $\lim_{|\boldsymbol{r}_i|\to\infty} V_i(\boldsymbol{r}_i)=\lim_{|\boldsymbol{r}_i-\boldsymbol{r}_j|\to\infty} V_{ij}(\boldsymbol{r}_i,\boldsymbol{r}_j)=0$ (theorem 7). For Coulomb systems a complete distinction of all possible cases is given in theorem 8.

In § 3 we conclude from scaling arguments that $E_i(R)\leqslant 0$ and $R\cdot E_i(R)$ is decreasing, where $E_i(R)$ denotes the ith eigenvalue of $H(R)=\Sigma-\Delta_i/m_i+\Sigma\, z_iz_j/|\boldsymbol{r}_i-\boldsymbol{r}_j|+\Sigma\, z_iZ_k/|\boldsymbol{r}_i-R\cdot\boldsymbol{R}_k|$ (theorem 10). The value of theorem 10 becomes obvious when one remembers that it is derived for the general case of arbitrary charges z_i and Z_k, while statements concerning the monotonicity of $E_1(R)$ explicitly depend on the kind of charges (cf remark 15). A simple special case of our theorem 10 has already been proved by Thirring (1979), who showed the monotonicity of $R^2E_1(R)$ for H_2^+ (Born–Oppenheimer approximation assumed). Hoffmann-Ostenhof (1980) and Lieb and Simon (1978) presented a proof for the increasing of $E_1(R)$ of H_2^+ and of an electron in a field of protons respectively. Lieb (1982) generalised the second proof to the energy $E_1(\boldsymbol{R}_1,\ldots,\boldsymbol{R}_m)$ of an electron in a field of m protons, where the positions of the protons cannot be mapped into each other by a similarity transformation.

We, however, show, transferring the proof by Hoffmann-Ostenhof to an electron in the field of a dipole, that $E_1(R)$ is strictly monotone decreasing for $R>R_c$ (lemma

16). As proved by Alvarez-Estrado and Galindo (1978), $R_c = 0.639\,415$ is the distance of the dipole for critical binding of the electron. Hunziker and Günther (1980) repeated this proof by a more elegant method, completing the approach by Brown and Roberts (1967).

With the help of a result by Munschy and Stébé (1973) we prove that in the dipole–exciton system there is (exactly one) other critical value $R > R_c$ for which the binding energy is non-analytic (lemma 18).

In § 4 we investigate the ground-state energy and excited-state energies of the biexciton for which Adamowski *et al* (1972) proved stable binding for all mass ratios σ. We overcome a weak point in their proof, simplify it by using concavity arguments, sharpen one conclusion and add a statement concerning $E^i(\sigma) = \Sigma_{j=1}^i E_j(\sigma)$ (theorem 19).

2. Monotonicity and concavity of energies

In the sequel H_0 and H' are self-adjoint operators with a common essential domain (cf Reed and Simon 1972, § 8.2). Let us denote by $E_i(\alpha)$, $\varphi_i(\alpha)$, the ith eigenvalue and the ith eigenvector of $H(\alpha) = H_0 + \alpha H'$, respectively (counting multiplicity, $\alpha \geqslant 0$), $E^i(\alpha) = \Sigma_{j=1}^i E_j(\alpha)$, $T_i(\alpha) = \langle \varphi_i(\alpha), H_0\varphi_i(\alpha)\rangle$, $T^i(\alpha) = \Sigma_{j=1}^i T_j(\alpha)$, $V_i(\alpha) = E_i(\alpha) - T_i(\alpha)$, $V^i(\alpha) = E^i(\alpha) - T^i(\alpha)$. If $H(\alpha)$ has only $k < i$ eigenvalues below the essential spectrum then put $E_{k+1}(\alpha) = E_{k+2}(\alpha) = \cdots = E_\infty(\alpha) := \inf \sigma_{\rm ess} H(\alpha)$. If $E_k = E_{k+1}$ choose φ_k orthogonal to φ_{k+1}.

Definition 1. $E(\alpha)$ is concave if for every λ with $0 \leqslant \lambda \leqslant 1$ and $\mu = 1 - \lambda$, $E(\lambda\alpha + \mu\beta) \geqslant \lambda E(\alpha) + \mu E(\beta)$.

Lemma 2. For arbitrary H_0, H' and $\alpha \geqslant 0$ it holds that $E^i(\alpha)$ is concave, $T^i(\alpha)$ is increasing and $V^i(\alpha)/\alpha$ is decreasing.

Proof. Since $H(\lambda\alpha + \mu\beta) = \lambda H(\alpha) + \mu H(\beta)$ we get

$$\begin{aligned} E^i(\lambda\alpha + \mu\beta) &= \sum_{j=1}^{i} \langle \varphi_j(\lambda\alpha + \mu\beta), H(\lambda\alpha + \mu\beta)\varphi_j(\lambda\alpha + \mu\beta)\rangle \\ &= \lambda \sum_j \langle \varphi_j(\lambda\alpha + \mu\beta), H(\alpha)\varphi_j(\lambda\alpha + \mu\beta)\rangle \\ &\quad + \mu \sum_j \langle \varphi_j(\lambda\alpha + \mu\beta), H(\beta)\varphi_j(\lambda\alpha + \mu\beta)\rangle \\ &\geqslant \lambda \sum_j \langle \varphi_j(\alpha), H(\alpha)\varphi_j(\alpha)\rangle + \mu \sum_j \langle \varphi_j(\beta), H(\beta)\varphi_j(\beta)\rangle = \lambda E^i(\alpha) + \mu E^i(\beta). \end{aligned}$$

The '$\geqslant$' sign follows from the min–max principle (cf e.g. Thirring 1979, § 3.5, 21) which yields

$$\sum_{j=1}^{i} E_j = \min_{\{\psi_j\}} \sum_{j=1}^{i} \langle \psi_j, H\psi_j\rangle \tag{1}$$

where the minimum is taken over all orthonormal systems $\{\psi_j\}$ with $j = 1, \ldots, i$. Thus the concavity is proved. Analogously, it holds that

$$E^i(\alpha) = T^i(\alpha) + V^i(\alpha) \leq \sum_{j=1}^{i} \langle \varphi_j(\beta), (H_0 + \alpha H')\varphi_j(\beta)\rangle = T^i(\beta) + (\alpha/\beta)V^i(\beta). \tag{2}$$

Conversely we get $E^i(\beta) = T^i(\beta) + V^i(\beta) \leq T^i(\alpha) + (\beta/\alpha)V^i(\alpha)$.

If $\alpha < \beta$ then the addition of these two inequalities yields

$$V^i(\alpha) + V^i(\beta) \leq (\alpha/\beta)V^i(\beta) + (\beta/\alpha)V^i(\alpha)$$

and

$$V^i(\beta)/\beta \leq V^i(\alpha)/\alpha. \tag{3}$$

From (2) and (3) we see

$$T^i(\beta) - T^i(\alpha) \geq V^i(\alpha) - (\alpha/\beta)V^i(\beta) \geq 0.$$

If $H(\lambda\alpha + \mu\beta)$ has only $k < i$ eigenvalues below the essential spectrum then for $j > k$ one can choose an orthonormal set of approximate eigenfunctions φ^j_ε with

$$E_j(\lambda\alpha + \mu\beta) \geq \langle \psi^j_\varepsilon(\lambda\alpha + \mu\beta), H(\lambda\alpha + \mu\beta)\varphi^j_\varepsilon(\lambda\alpha + \mu\beta)\rangle - \varepsilon.$$

Then $E^i(\lambda\alpha + \mu\beta) \geq \lambda E^i(\alpha) + \mu E^i(\beta) - \varepsilon$ for arbitrary $\varepsilon > 0$, and hence concavity is proved also in this case. We complete the proof for T^i and V^i analogously.

Remark 3. The concavity of $E^i(\alpha)$ is a well known property (cf e.g. Thirring 1979, § 3.5, 23). For further useful concavity properties, cf Thirring (1979, § 4.3, 19 and § 4.6, 4). If $E^i(\alpha)$ is differentiable then the monotonicity of $T^i(\alpha)$ can also be obtained with the help of the Feynman–Hellmann relation $\mathrm{d}E^i(\alpha)/\mathrm{d}\alpha = V^i(\alpha)/\alpha$ and the concavity condition of $E^i(\alpha)$, which is for twice differentiable functions equivalent to $\mathrm{d}^2E^i(\alpha)/\mathrm{d}^2\alpha \leq 0$. Thus

$$\mathrm{d}T^i(\alpha)/\alpha = \mathrm{d}(E^i(\alpha) - \alpha\ \mathrm{d}E^i(\alpha)/\mathrm{d}\alpha)/\mathrm{d}\alpha = -\alpha\ \mathrm{d}^2E^i(\alpha)/\mathrm{d}^2\alpha \geq 0.$$

This approach was used by Misawa (1968) in his monotonicity proof for $T_1(\alpha)$. In addition, he had to assume the applicability of perturbation theory since the concavity condition used by him is based on it in the following manner. Let $(\alpha_0 - \alpha)H'$ be a perturbation of $H(\alpha) = H_0 + \alpha H'$ which has the unperturbed eigenfunctions $\varphi_i^{(0)}(\alpha)$ and eigenvalues $E_i^{(0)}(\alpha)$. Perturbation theory yields $E_1(\alpha_0) = \Sigma_{k=0}^{\infty}(\alpha_0 - \alpha)^k E^{(k)}(\alpha)$ with $E^{(2)}(\alpha) = \Sigma_{i\neq 1}\langle \varphi_1^{(0)}, H'\varphi_i^{(0)}\rangle^2/(E_1^{(0)} - E_i^{(0)}) < 0$. Then

$$\mathrm{d}^2E_1(\alpha_0)/\mathrm{d}\alpha^2_{0|\alpha_0=\alpha} = 2E^{(2)}(\alpha) < 0.$$

But as has been shown above, the concavity of $E^i(\alpha)$ and the monotonicity of $T^i(\alpha)$ can be concluded independently of the applicability of perturbation theory and of differentiability conditions.

Lemma 4. If $\gamma < \alpha < \beta$ and $E^i(\alpha) \leq E^i(\gamma)$ then $E^i(\beta) \leq E^i(\alpha)$ and $V^i(\beta) \leq V^i(\alpha)$ (i.e. E^i and V^i are monotone decreasing functions). If $E^i(\alpha) < E^i(\gamma)$ then $E^i(\beta) < E^i(\alpha)$ and $V^i(\beta) < V^i(\alpha)$ (i.e. E^i and V^i are strictly monotone decreasing functions).

Proof. Put $\lambda = (\alpha - \beta)/(\gamma - \beta)$. With the help of lemma 2 we conclude

$$\begin{aligned} E^i(\alpha) &= E^i(\lambda\gamma + \mu\beta) \geq \lambda E^i(\gamma) + \mu E^i(\beta) \geq \lambda E^i(\alpha) + \mu E^i(\beta) \\ &= (\alpha - \beta)E^i(\alpha)/(\gamma - \beta) + (\gamma - \alpha)E^i(\beta)/(\gamma - \beta). \end{aligned} \tag{4}$$

Thus $E^i(\alpha)\geqslant E^i(\beta)$. If $E^i(\gamma)>E^i(\alpha)$ one gets a '>' sign in the last inequality of (4) and hence $E^i(\alpha)>F^i(\beta)$. If $E^i(\alpha)$ is (strictly) monotone decreasing then $V^i(\alpha)=E^i(\alpha)-T^i(\alpha)$ is also (strictly) monotone decreasing since, by lemma 2, $T^i(\alpha)$ is always increasing.

From the monotonicity of $E^i(\alpha)$ one cannot conclude the monotonicity of $E_i(\alpha)$ for $i>1$ (cf Thirring 1979, § 3.5, 25). The monotonicity of $E_i(\alpha)$ is only derivable under further restrictions.

Lemma 5. If $E_i(\alpha)\leqslant E_1(0)$ and $0<\alpha<\beta$ then $E_i(\beta)$ is monotone decreasing, $(E_i(\beta)-E_1(0))/\beta\leqslant(E_i(\alpha)-E_1(0))/\alpha$, $V_i(\alpha)\leqslant 0$ and $V^i(\beta)$ is at least linearly monotone decreasing (i.e. $V^i(\beta_2)\leqslant V^i(\beta_1)$ and $V^i(\beta_2)/\beta_2\leqslant V^i(\beta_1)/\beta_1$ for $\alpha<\beta_1<\beta_2$). If $E_i(\alpha)<E_1(0)$ then $E_i(\beta)$ is strictly monotone decreasing, $V_i(\alpha)<0$ and $V^i(\beta)$ is at least linearly strictly monotone decreasing (i.e. $V^i(\beta_2)<V^i(\beta_1)$ and $V^i(\beta_2)/\beta_2\leqslant V^i(\beta_1)/\beta_1$ for $\alpha<\beta_1<\beta_2$).

Remark 6. The monotonicity of $E_i(\beta)$ has been proved in Reed and Simon (1978, p 79), under the additional assumption $\sigma_{\text{ess}}H(\alpha)=[0;\infty)$. But in systems with more than one light particle in general it holds that $\sigma_{\text{ess}}H(\alpha)<0$, i.e. for these systems the version by Reed and Simon is not applicable. The condition of lemma 5 does not imply the concavity of $E_i(\alpha)$ for $i\geqslant 2$, as already simple examples of diagonal 2×2 matrices show.

Proof of lemma 5. Let $\mathcal{H}_i$ be an arbitrary i-dimensional subspace and

$$\mathcal{H}_i(\alpha)=\left\{\varphi\,\middle|\,\varphi=\sum_{j=1}^{i}\lambda_j\varphi_j(\alpha),\ \|\varphi\|=1,\ \lambda_j\in R\right\}.$$

From the min–max principle

$$E_i=\min_{\mathcal{H}_i}\ \max_{\varphi\in\mathcal{H}_i,\|\varphi\|=1}\langle\varphi, H\varphi\rangle \tag{5}$$

and $\langle\varphi,(H(0)-E_1(0))\varphi\rangle\geqslant 0$ for all φ follows

$$\begin{aligned}(E_i(\beta)-E_1(0))/\beta &\leqslant \max_{\varphi\in\mathcal{H}_i(\alpha)}\langle\varphi,((H(0)-E_1(0))/\beta+H')\varphi\rangle\\ &\leqslant \max_{\varphi\in\mathcal{H}_i(\alpha)}\langle\varphi,((H(0)-E_1(0))/\alpha+H')\varphi\rangle\\ &=(E_i(\alpha)-E_1(0))/\alpha.\end{aligned} \tag{6}$$

The assumption $E_i(\alpha)\leqslant E_1(0)$ yields

$$(E_i(\alpha)-E_1(0))/\alpha\leqslant(E_i(\alpha)-E_1(0))/\beta \tag{7}$$

and therefore, in connection with (6), it holds that $E_1(\beta)\leqslant E_1(\alpha)$.

Now obviously $E_i(\beta)\leqslant E_1(0)$ and we can repeat the proof putting $\alpha=\beta_1$ and $\beta=\beta_2$. Thus the monotonicity of $E_i(\beta)$ has been shown. The assumption also yields

$$\begin{aligned}V_i(\alpha)=E_i(\alpha)-T_i(\alpha)&=E_i(\alpha)-\langle\varphi_i(\alpha),H(0)\varphi_i(\alpha)\rangle\\ &\leqslant E_i(\alpha)-\langle\varphi_1(0),H(0)\varphi_1(0)\rangle\leqslant 0.\end{aligned}$$

From this relation and inequality (3) we see that $V^i(\beta_2)\leqslant\beta_2V^i(\beta_1)/\beta_1\leqslant V^i(\beta_1)$ which satisfy our definition of linear monotonicity. If $E_i(\alpha) < E_1(0)$ then $(E_1(\alpha) - E_1(0))/\alpha < (E_i(\alpha) - E_1(0))/\beta$, $E_i(\beta) < E_i(\alpha)$ and therewith $E_i(\beta_2) < E_i(\beta_1)$, $V_i(\alpha) < 0$. If $H(\alpha)$ has only $k < i$ eigenvalues below the essential spectrum then we proceed in the same manner as in the proof of lemma 2.

In the following the notation 'light' and 'heavy' particles is used for particles described in the Born–Oppenheimer approximation with masses $m < \infty$ and $m = \infty$, respectively. Light particles have the charges z_i and the positions $\boldsymbol{r}_i$, heavy particles have Z_i and $\boldsymbol{R}_i$.

Now we can introduce the main theorem.

Theorem 7. Let $H(\alpha) = H_0 + \alpha H'$ with $H_0 = \Sigma_{i=1}^{n} - \Delta_i/m_i$ and

$$H' = \sum_{j=2}^{n} \sum_{i=1}^{j-1} z_i z_j / |\boldsymbol{r}_i - \boldsymbol{r}_j| + \sum_{i=1}^{n} \sum_{k=1}^{m} z_i Z_k / |\boldsymbol{r}_i - \boldsymbol{R}_k|. \tag{8}$$

Then for all i and all $\alpha \geq 0$ it holds that: $E^i(\alpha)$ is concave. $T^i(\alpha)$ increases monotonely. $E_i(\alpha)$—and hence also $E^i(\alpha)$—is an at least linearly monotone decreasing function. $V^i(\alpha)$ is an at least linearly monotone decreasing function.

Proof. The concavity of $E^i(\alpha)$ and the monotonicity of $T^i(\alpha)$ immediately follow from lemma 2. The linear monotonicity of $E_i(\alpha)$ and $V^i(\alpha)$ can be concluded from lemma 5, since our Hamiltonian (8) satisfies the assumption

$$E_i(\alpha) \leq E_1(0) = 0. \tag{9}$$

We take for every $\varepsilon > 0$ a normalised test-function φ_ε^i, orthogonal to the first $(i-1)$ eigenvectors, which describes the following situation. All light particles have a sufficiently small kinetic energy and are sufficiently far away from all $\boldsymbol{R}_i$ and from each other. The min–max principle (cf (5)) yields

$$E_i(\alpha) \leq \langle \varphi_\varepsilon^i, (H_0 + \alpha H')\varphi_\varepsilon^i \rangle < \varepsilon \tag{10}$$

for arbitrarily small ε. Thus $E_i(\alpha) \leq 0$ and therewith the linear monotonicity of $V^i(\alpha)$ and $E_i(\alpha)$ is proved. If $H(\alpha)$ has only $k < i$ eigenvalues below the essential spectrum then the above proof shows $E_{k+1}(\alpha) \leq 0$. Per definition we then have $E_i(\alpha) = E_{k+1}(\alpha) \leq 0$.

Theorem 7 comprises the following three cases. In the last two cases the propositions concerning the monotonicity of $E_i(\alpha)$ and $V^i(\alpha)$ can be sharpened.

Theorem 8.

(a) If all particles have charges of the same sign then $V_i(\alpha) = T_i(\alpha) = E_i(\alpha) = 0$.

(b) If there is at least one pair of oppositely charged heavy particles and all light particles have charges of the same sign, then there is for every i an α_i such that $E_i(\alpha)$ and $V^i(\alpha)$ are at least linearly strictly monotone decreasing for $\alpha \geq \alpha_i$. (A typical example is the electron bound to a dipole, cf e.g. Alvarez-Estrado and Galindo (1978).)

(c) In all other configurations $E_i(\alpha)$ and $V^i(\alpha)$ are at least linearly strictly monotone decreasing for $\alpha \geq 0$. (Typical examples are: H_2 and H_2^+ in Born–Oppenheimer approximation, $D^+ + A^- +$exc in effective-mass approximation (D^+ denotes a donor, A^- an acceptor, exc an exciton consisting of an electron e^- and a positively charged hole h^+).)

Proofs.

(a) If all charges have the same sign then $V_i(\alpha) \geq 0$ and therefore we get $E_i(\alpha) \geq E_1(0) + V_i(\alpha) \geq E_1(0) = 0$. Together with (9) this implies $E_i(\alpha) = 0$. From $V_i(\alpha) \geq 0$ and $V_i(\alpha) \leq 0$ (by lemma 5) we see $V_i(\alpha) = T_i(\alpha) = 0$.

(b) For every $\varepsilon > 0$ one can find a test function φ^i_ε, orthogonal to the first $(i-1)$ eigenvectors, which describes one light particle (e.g. that with index 1) as being so closely bound to one of the heavy particles having an opposite charge to it, that

$$\tilde{V} = \left\langle \varphi^i_\varepsilon, \sum_{k=1}^{m} z_1 Z_k / |\boldsymbol{r}_1 - \boldsymbol{R}_k| \varphi^i_\varepsilon \right\rangle < 0.$$

The other light particles are described as having a sufficiently small kinetic energy and as being far away from all $\boldsymbol{R}_k$ and from each other. Thus we only have to consider the kinetic energy $T = \langle \varphi^i_\varepsilon, (-\Delta_1/m_1)\varphi^i_\varepsilon \rangle$ (which can be very high due to the localisation) and the potential energy $\alpha\tilde{V}$. Obviously there exists an α_i such that for all $\alpha \geq \alpha_i$, $E_i(\alpha) \leq \langle \varphi^i_\varepsilon, (H_0 + \alpha H')\varphi^i_\varepsilon \rangle = \tilde{T} + \alpha\tilde{V} + \varepsilon < 0$. Now lemma 5 yields the linear monotonicity of $E_i(\alpha)$ and $V^i(\alpha)$ for $\alpha \geq \alpha_i$.

(c) All other configurations can be reduced to two cases.

(c1) All heavy particles have charges of the same sign and at least one light particle has the opposite charge to this. Let $z_1 Z_i < 0$ for all i. We choose test functions φ^i_ε consisting of the hydrogen-like solutions of the Hamiltonian $-\Delta_1/m_1 + \alpha z_1 Z_1/|\boldsymbol{r}_1 - \boldsymbol{R}_1|$, multiplied by a function describing all other light particles as having a sufficiently small kinetic energy and as being far away from each other and from all $\boldsymbol{R}_i$. Then $E_i(\alpha) \leq \langle \varphi^i_\varepsilon, H(\alpha)\varphi^i_\varepsilon \rangle \leq -m_1(\alpha z_1 Z_1/2i)^2 + \varepsilon$ for all $\varepsilon > 0$. Thus $E_i(\alpha) < 0$ for all $\alpha > 0$ and lemma 5 yields the linear strict monotonicity of $E_i(\alpha)$ and $V^i(\alpha)$ for $\alpha \geq 0$.

(c2) The heavy particles are arbitrarily charged and at least two light particles have charges of opposite sign to each other. Let $z_1 z_2 < 0$. We get our test function φ^i_ε by multiplying the hydrogen-like solutions of the Hamiltonian $-\Delta_1/m_1 - \Delta_2/m_2 + \alpha z_1 z_2/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ by a function describing the other light particles and the centre of gravity of the first two particles as having small kinetic energy and as being far away from each other and from all $\boldsymbol{R}_i$. For every $\varepsilon > 0$ it holds that

$$E_i(\alpha) \leq \langle \varphi^i_\varepsilon, H(\alpha)\varphi^i_\varepsilon \rangle = -\mu(\alpha z_1 z_2/2i)^2 + \varepsilon \qquad \text{with} 1/\mu = 1/m_1 + 1/m_2.$$

Analogously to case (c1) we can now conclude the linear strict monotonicity of $E_i(\alpha)$ and $V^i(\alpha)$ for $\alpha \geq 0$.

If $H(\alpha)$ has only $k < i$ eigenvalues below the essential spectrum then we proceed in the cases (b) and (c) in the same manner as in the proof of theorem 7.

Remark 9. The proofs of theorems 7 and 8 are related to the proof of the trivial part of the HVZ-theorem (cf Reed and Simon 1978, p 122). Hence, one can also prove theorem 7 and, for $n \geq 2$, theorem 8 by applying the HVZ-theorem, instead of the min–max principle. In case (b) the HVZ-theorem additionally yields that $\sup_i \alpha_i < \infty$ or—in other words—that $E_\infty(\alpha)$ becomes negative: $E_i(\alpha) \leq E_\infty(\alpha) \leq \inf \sigma(-\Delta_1/m_1 + \alpha \sum z_1 Z_k/|\boldsymbol{r}_1 - \boldsymbol{R}_k|) < 0$ for sufficiently large α.

3. The $\boldsymbol{E}(\boldsymbol{R})$ dependence

Often of interest is the case where not only the coupling constant α but also the distance between the heavy particles varies. The Hamiltonian for such a Coulomb system can be written in the general form

$$H(\varepsilon, m, R) = H_0(m) + H'(R)/\varepsilon \qquad \text{with } H_0(m) = \sum_{i=1}^{n} -\Delta_i/(m \cdot m_i)$$

and

$$H'(R) = \sum_{j=2}^{n}\sum_{i=1}^{j-1} z_i z_j/|\boldsymbol{r}_i - \boldsymbol{r}_j| + \sum_{i=1}^{n}\sum_{k=1}^{m} z_i Z_k/|\boldsymbol{r}_i - R\cdot \boldsymbol{R}_k|, \tag{11}$$

where ε is the dielectric constant. $E_i(\varepsilon, m, R)$ denotes the ith eigenvalue of (11); if we keep m and ε constant we write shortly $E_i(R)$. ($E_i(m)$ and $E_i(\varepsilon)$ are defined analogously.)

First (theorem 10) we derive some results concerning $R^2E_i(R)$ and $RE_i(R)$ for all Hamiltonians of the form (11). In lemma 12 we deal with the complete Born–Oppenheimer energy $E_i^c(\varepsilon, m, R)$ (including the Coulomb interaction between the heavy particles). Lastly we present statements regarding $E_1(R)$ in some special cases. (Of course the following results are only non-trivial if at least two heavy particles are present.)

Theorem 10. All statements of theorems 7 and 8 are valid for the Hamiltonian (11) if $E_i(\alpha)$ is replaced by $R^2E_i(R)$ or $mE_i(m)$ or $E_i(\varepsilon)$ as a function of $1/\varepsilon$. In particular that means:

(i) $E_i(\varepsilon, m, R) \leq 0$;
(ii) $mE_i(m)$ and $R^2E_i(R)$ are decreasing and $E_i(\varepsilon)$ is increasing;
(iii) $E_i(m)$ and $RE_i(R)$ are decreasing and $\varepsilon E_i(\varepsilon)$ is increasing;
(iv) $mE^i(m)$, $R^2E^i(R)$ and $\varepsilon E^i(\varepsilon)$ are concave.

Proof. Substitute $\boldsymbol{r}_i \to R\boldsymbol{r}_i$. Then

$$E_i(\varepsilon, m, R) = E_i(H_0(m) + H'(R)/\varepsilon) = E_i(H_0(m)/R^2 + \Sigma z_i z_j/(|\boldsymbol{r}_i - \boldsymbol{r}_j|\varepsilon R)$$
$$+ \Sigma z_i Z_k/(|\boldsymbol{r}_i - \boldsymbol{R}_k|\varepsilon R)) = (mR^2)^{-1}E_i(H_0(1) + mR\cdot H'(1)/\varepsilon).$$

Putting $\alpha = mR/\varepsilon$ it is obvious that $H_0(1) + mR\cdot H'(1)/\varepsilon = H(\alpha)$, as defined in (8). Since theorems 7 and 8 were proved for (8), their statements must also be valid for $mR^2E_i(\varepsilon, m, R)$ and—keeping constant two variables at a time—also for $E_i(\varepsilon)$, $mE_i(m)$ and $R^2E_i(R)$. Now the linear decrease of $E_i(\varepsilon)$, $mE_i(m)$ and $R^2E_i(R)$ with respect to $1/\varepsilon$, m and R, respectively (theorem 7), immediately yields the increase of $\varepsilon E_i(\varepsilon)$ and the decrease of $E_i(m)$ and $RE_i(R)$. The easiest way to get the concavity of $\varepsilon E^i(\varepsilon)$ is the direct application of lemma 2 to $\varepsilon H_0 + H' = \varepsilon H(\varepsilon)$.

Remark 11. A simple special case of theorem 10 has already been proved by Thirring (1979, §4.6, 24), who showed the monotonicity of $R^2E_1(R)$ for H_2^+. (He did need the strong restriction $H'(1) \leq 0$.)

Lemma 12. For the energy $E_i^c(\varepsilon, m, R)$ of the complete Born–Oppenheimer Hamiltonian

$$H^c(\varepsilon, m, R) = H(\varepsilon, m, R) + \sum_{i=2}^{m}\sum_{k=1}^{i-1} Z_i Z_k/(|\boldsymbol{R}_i - \boldsymbol{R}_k|\varepsilon R) \tag{12}$$

(which includes the Coulomb interaction between the heavy particles) it holds that

(i) $\varepsilon E^{c,i}(\varepsilon)$, $mE^{c,i}(m)$ and $R^2E^{c,i}(R)$ are concave;

(ii) $E_i^c(m)$ and $RE_i^c(R)$ are decreasing and $\varepsilon E_i^c(\varepsilon)$ is increasing;

(iii) if $\Sigma Z_i Z_k/|\boldsymbol{R}_i - \boldsymbol{R}_k| < 0$, then $E_i^c(\varepsilon, m, R) < 0$; $mE_i^c(m)$ and $R^2 E_i^c(R)$ are strictly decreasing and $E_i^c(\varepsilon)$ is strictly increasing.

Proof. From (12) it is obvious that

$$E_i^c(\varepsilon, m, R) = E_i(\varepsilon, m, R) + \Sigma Z_i Z_k/(|\boldsymbol{R}_i - \boldsymbol{R}_k|\varepsilon R).$$

Now assertion (i) follows from theorem 10(iv) and the fact that the sum of a concave and a linear function is concave. Theorem 10(iii) yields our assertion (ii), since $\Sigma Z_i Z_k/|\boldsymbol{R}_i - \boldsymbol{R}_k|$ is a constant and therefore it cannot change the monotonicity. If this constant is less than zero, then by theorem 10(i) $E_i^c(\varepsilon, m, R) < 0$ which yields in connection with lemma 5 and theorem 10 the assertion (iii). We can also prove (iii) remembering that in the case considered $mR\,\Sigma Z_i Z_k/(|\boldsymbol{R}_i - \boldsymbol{R}_k|\varepsilon)$ is strictly decreasing with respect to mR/ε and that the sum of a decreasing and a strictly decreasing function is strictly decreasing.

Remark 13. In the following we only consider systems consisting of two heavy particles. Let them have the coordinates (0; 0; 0) and (1; 0; 0) respectively such that the scaling factor R from (11) immediately denotes the distance of the heavy particles. Let $\boldsymbol{R}$ be the vector $(R; 0; 0)$. Then (11) reads

$$H(\varepsilon, m, R) = \sum_{i=1}^{n} -\frac{\Delta_i}{(mm_i)} + \left(\sum_{j=2}^{n} \sum_{i=1}^{j-1} \frac{z_i z_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_{i=1}^{n} z_i \left(\frac{Z_1}{r_i} + \frac{Z_2}{|\boldsymbol{r}_i - \boldsymbol{R}|} \right) \right) \Big/ \varepsilon. \tag{13}$$

Of course, theorem 10 also applies to (13).

Remark 14. If the system $D^+ + A^- + \mathrm{exc}$ is treated in effective-mass approximation, its Hamiltonian can be written in the form (13) with $z_1 = -z_2 = -Z_1 = Z_2 = -|e|$. Therefore the energies $E_i(\varepsilon, m, R)$ of this system satisfy all statements of theorem 10. But the Coulomb approximation (cf Bindemann and Unger 1973) which yields

$$E_1(\varepsilon, m, R) = \sum_{i=1}^{2} (-mm_i e^4/(2\varepsilon^2)) + e^2/(\varepsilon R) \tag{14}$$

violates statements (i) and (ii) of theorem 10 as well as case (c) of theorem 8 when either $1/\varepsilon$, m or R is small. It is well known that the Coulomb approximation only gives good values for large R; here we have shown that it yields a *qualitatively* wrong behaviour of the energy.

It is not possible to get such strong results regarding $E(R)$ for the large class of Hamiltonians described by (11). Remark 15 and lemma 16 contain some statements for $E_1(R)$ in special cases of (11).

Remark 15. Narnhofer and Thirring (1975) proved that if in (11) all $z_i < 0$, all $Z_k > 0$ then $E_1(R) > E_1(0)$. Lieb and Simon (1978) showed for $n = 1$, $z_1 < 0$, all $Z_k > 0$ that $E_1(R)$ is monotone increasing. (For $m = 2$ there is also another proof for the same statement by Hoffmann-Ostenhof (1980).)

Lieb (1982) derived a stronger result for the same case. If there are two sets $\{\boldsymbol{R}_i\}$, $\{\boldsymbol{R}'_i\}$ with $|\boldsymbol{R}_i - \boldsymbol{R}_j| \geq |\boldsymbol{R}'_i - \boldsymbol{R}'_j|$ for all pairs i, j then $E_1(\{\boldsymbol{R}_i\}) \geq E_1(\{\boldsymbol{R}'_i\})$.

In the following we prove that the ground-state energy of an electron bound to a dipole of distance R is strictly monotone decreasing for $R \geq R_c$, where R_c denotes the critical distance for which it holds that the system is stable for $R > R_c$ and unstable for $R \leq R_c$. Alvarez-Estrado and Galindo (1978) proved in the case $mm_1 = 1/2$, $Z_1 = -Z_2$ that

$$R_c = 0.639\,415/|\varepsilon^{-1} z_1 Z_1|. \tag{15}$$

Lemma 16. If in (13) $n = 1$, $Z_1 > 0$, $Z_2 < 0$ then $E_1(R)$ is a strictly decreasing function for $R \geq R_c$.

Proof. We transfer the proof by Hoffmann-Ostenhof (1980) for the monotonicity of the H_2^+ molecule to our problem. Let $mm_1 = \frac{1}{2}$, $\varepsilon = 1$ and $z_1 < 0$; the oppositely charged heavy particle has the coordinates (0; 0; 0), the equally charged one the coordinates (R; 0; 0). After applying the Feynman–Hellmann relation for $R > R_c$ (due to theorems 12.8 and 13.46 in Reed and Simon (1978) all stable ground-state energies are differentiable!) we divide the integration over x into an integration from $-\infty$ to R and from R to ∞ and substitute in the first integral $x \to 2R - x$:

$$\begin{aligned} \mathrm{d}E_1(R)/\mathrm{d}R &= -z_1 Z_2 \iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, (x - R)|\boldsymbol{r} - \boldsymbol{R}|^{-3} \varphi_1^2(R, x, y, z) \\ &= z_1 Z_2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}y\, \mathrm{d}z \int_R^{\infty} \mathrm{d}x (R - x)|\boldsymbol{r} - \boldsymbol{R}|^{-3} \\ &\quad \times (\varphi_1^2(R, 2R - x, y, z) - \varphi_1^2(R, x, y, z)). \end{aligned} \tag{16}$$

From theorem 2.1 in Hoffmann-Ostenhof (1980) we see $\varphi_1^2(R, 2R - x, y, z) \geq \varphi_1^2(R, x, y, z)$, since our definitions $W := z_1 Z_1/r + z_1 Z_2/|\boldsymbol{r} - \boldsymbol{R}| - E_1(R)$ (potential for $x \geq R$), $V := z_1 Z_1/|\boldsymbol{r} - 2\boldsymbol{R}| + z_1 Z_2/|\boldsymbol{r} - \boldsymbol{R}| - E_1(R)$ (potential for $x \leq R$) yield

$$W > V. \tag{17}$$

$\varphi_1^2(R, 2R - x, y, z) \equiv \varphi_1^2(R, x, y, z)$ is not possible, since this would imply $W \equiv V$ in contradiction to (17). Therefore the integration in (16) gives a negative result (remember that $z_1 Z_2 > 0$ and $R - x < 0$) and we get

$$\mathrm{d}E_1(R)/\mathrm{d}R < 0. \tag{18}$$

Remark 17. With our last arguments it is at once possible to extend the proof by Hoffmann-Ostenhof (1980) for the monotonicity of the H_2^+ molecule to strict monotonicity. This extension was also presented by a related argument in Hoffmann-Ostenhof and Morgan (1981).

Now we return to the system $D^+ + A^- +$exc and give a statement for its binding energy (calculated in effective-mass approximation) $E_B(R) = E_1(R) - E_\infty(R)$ where $E_\infty(R) = \inf \sigma_{ess} H(R)$.

Lemma 18. If in (13) $n = 2$, $z_1 = -z_2 = -Z_1 = Z_2 = -|e|$ then the binding energy $E_B(R) = E_1(R) - E_\infty(R)$, for $E_B(R) < 0$, has a cusp (i.e. a discontinuous first derivative) at exactly one point.

Proof. In (13), put $m = m_1 = 1$, $m_2 = m_1/\sigma$, $e^2/\varepsilon = 2$. Then the Hamiltonian for the system under consideration reads

$$H(R) = -\Delta_1 - \sigma\Delta_2 - 2/|\boldsymbol{r}_1 - \boldsymbol{r}_2| + 2/r_1 - 2/|\boldsymbol{r}_1 - \boldsymbol{R}| + 2/|\boldsymbol{r}_2 - \boldsymbol{R}| - 2/r_2. \tag{19}$$

Due to the symmetry of this problem ($E(\sigma)=E(1/\sigma)/\sigma$) we restrict our considerations to $\sigma \geqslant 1$.

Munschy and Stébé (1973) sketched a proof for the stability of this system for $R>R_c=0.639415$, i.e. $E_B(R)<0$ for $R>R_c$. The complex $D^+ + A^- +$exc can dissociate into the two subsystems $D^+ + A^- + e^-$ (whose ground-state energy shall be $E_1^e(R)$) and h^+, which yields the dissociation energy

$$E_B^I(R)=E_1(R)-E_1^e(R) \tag{20}$$

or into the two subsystems $D^+ + A^-$ and exc, which yields the dissociation energy

$$E_B^{II}(R)=E_1(R)+1/(1+\sigma). \tag{21}$$

If $E_1^e(R)<-1/(1+\sigma)$ the first possibility will occur, if $E_1^e(R)>-1/(1+\sigma)$ the second one. Since, with respect to R, $-1/(1+\sigma)$ is a constant lying between $-\frac{1}{2}$ and 0 and since $E_1^e(R)$ is (due to lemma 16) strictly monotone decreasing between $E_1^e(R_c)=0$ and $E_1^e(\infty)=-1$, there is for every $\sigma<\infty$ exactly one $\bar{R}>R_c$ such that $-1/(1+\sigma)=E_1^e(\bar{R})$. Therefore

$$E_B(R)=\begin{cases} E_B^{II}(R) & \text{for } R\leqslant \bar{R} \\ E_B^I(R) & \text{for } R>\bar{R}. \end{cases} \tag{22}$$

Equations (20), (21) and lemma 16 yield

$$\mathrm{d}E_B^I(R)/\mathrm{d}R_{|R=\bar{R}}-\mathrm{d}E_B^{II}(R)/\mathrm{d}R_{|R=\bar{R}}=-\mathrm{d}E_1^e(R)/\mathrm{d}R_{|R=\bar{R}}>0.$$

Thus the binding energy $E_B(R)$ must possess a discontinuous first derivative at $R=\bar{R}$. For $E_B(R)<0$, $\bar{R}$ is the only point with this property, since then $E_B^{II}(R)$ for $R<\bar{R}$ and $E_B^I(R)$ for $R>\bar{R}$ are analytic functions (due to theorems 12.8 and 13.46 in Reed and Simon (1978)).

From the calculations by Wallis *et al* (1960) we find for $\sigma=1$, $\bar{R}=3.86$ and the discontinuity in the first derivative of $E_B(R)$ at $R=\bar{R}$ is about 0.11.

4. The biexciton

Adamowski *et al* (1972) showed that the Hamiltonian

$$H(\sigma)=-1/(1+\sigma)\cdot(\Delta_1+\Delta_2+\sigma\Delta_3+\sigma\Delta_4)+2/r_{12}+2/r_{34}-2/r_{13}-2/r_{14}-2/r_{23}-2/r_{24} \tag{23}$$

(describing the biexciton in effective-mass approximation) has for every σ a stable ground state if we regard the system after the separation of the centre of gravity. (This can be carried out as in Thirring (1979, § 4.6, 1). Without the separation, (23) has no discrete spectrum.) σ denotes the ratio 'electron masses ($m_1=m_2$) : hole masses ($m_3=m_4$)'; $r_{ij}=|\boldsymbol{r}_i-\boldsymbol{r}_j|$. Equation (23) enables us to measure all energies in units of the free exciton. The system is invariant with respect to an interchange of the indices $\{1;2\}\leftrightarrow\{3;4\}$, therefore

$$H(\sigma)\cong H(1/\sigma). \tag{24}$$

The following theorem is (mainly) equivalent to that by Adamowski *et al* (1972), but we sharpen one conclusion and overcome a weak point (cf remark 20), we simplify the proof and add a statement concerning $E^i(\sigma)$ for $i>1$.

Theorem 19. Equation (23) has (after the separation of the centre of gravity) a stable ground state for all σ. $E^i(\sigma)$ is increasing and concave for all $\sigma \in [0; 1]$ and decreasing for $\sigma \in [1; \infty)$.

Proof. Put $\alpha = \sigma/(1+\sigma)$. Then $\bar{H}(\alpha) = \bar{H}(0) + \alpha(\Delta_1 + \Delta_2 - \Delta_3 - \Delta_4)$ with

$$\bar{H}(0) = -\Delta_1 - \Delta_2 + 2/r_{12} + 2/r_{24} - 2/r_{13} - 2/r_{14} - 2/r_{23} - 2/r_{24}. \tag{25}$$

Equation (24) now reads

$$\bar{H}(\alpha) \cong \bar{H}(1-\alpha) \tag{26}$$

which obviously also follows from (25). Lemma 2 and (26) yield

$$\bar{E}^i(1/2) \geqslant \bar{E}^i(\alpha)/2 + \bar{E}^i(1-\alpha)/2 = \bar{E}^i(\alpha). \tag{27}$$

Thus the assumption of lemma 4 is satisfied and in connection with (26) we get: $\bar{E}^i(\alpha)$ is decreasing for $1 \geqslant \alpha \geqslant \frac{1}{2}$ and increasing for $0 \leqslant \alpha \leqslant \frac{1}{2}$.

Remembering that $\alpha = \sigma/(1+\sigma)$ is with respect to σ a monotone increasing function, from the monotonicity of $\bar{E}^i(\alpha)$ in the intervals $[0; 1/2]$ and $[1/2; 1]$, it immediately follows that $E^i(\sigma)$ is monotone increasing for $\sigma \in [0; 1]$ and monotone decreasing for $\sigma \in [1; \infty)$.

The concavity of $\bar{E}^i(\alpha)$ implies that for all $\alpha \in [\alpha_1; \alpha_2]$ and arbitrary $\alpha_1 < \alpha_2$, $\bar{E}^i(\alpha)$ lies above the straight line which goes through the points $(\alpha_1; \bar{E}^i(\alpha_1))$ and $(\alpha_2; \bar{E}^i(\alpha_2))$. This follows directly from definition 1, putting $\alpha = \alpha_1$, $\beta = \alpha_2$ and $\lambda = (\alpha_2 - \alpha)/(\alpha_2 - \alpha_1)$:

$$\bar{E}^i(\alpha) \geqslant (\alpha_2 \bar{E}^i(\alpha_1) - \alpha_1 \bar{E}^i(\alpha_2) + \alpha(\bar{E}^i(\alpha_2) - \bar{E}^i(\alpha_1)))/(\alpha_2 - \alpha_1).$$

Rewriting this in terms of σ we get

$$E^i(\sigma) \geqslant \frac{\sigma_2 E^i(\sigma_1)/(1+\sigma_2) - \sigma_1 E^i(\sigma_2)/(\sigma_1 + 1) + \sigma(E^i(\sigma_2) - E^i(\sigma_1))/(1+\sigma)}{\sigma_2/(1+\sigma_2) - \sigma_1/(1+\sigma_1)} \tag{28}$$

for all $\sigma \in [\sigma_1; \sigma_2]$ and arbitrary $\sigma_1 < \sigma_2$. The right-hand side of (28) describes for $\sigma > -1$ and

$$E^i(\sigma_2) - E^i(\sigma_1) \geqslant 0 \tag{29}$$

the concave branch of a hyperbola going through the points $(\sigma_1; E^i(\sigma_1))$ and $(\sigma_2; E^i(\sigma_2))$. Expression (29) is satisfied for $0 \leqslant \sigma_1 < \sigma_2 \leqslant 1$. Together with (28) this implies that $E^i(\sigma)$ is itself a concave function for all $\sigma \in [0; 1]$.

Sharma (1968a) proved with the help of trial functions that $\bar{E}_1(1/2) < -2$. Due to (27) this implies $\bar{E}_1(\alpha) < -2$ for all α, and therefore for all σ

$$E_1(\sigma) < -2. \tag{30}$$

If we can show that the essential spectrum of (23) (after the separation of the centre of gravity) does not begin below -2, then (30) proves the stability of the biexciton for all σ. From the physical point of view it is clear that a biexciton dissociates into two free excitons, which corresponds to the essential spectrum beginning at -2, and does not dissociate into a hole and an $e^-e^-h^+$ complex, since the electron is more strongly bounded to the positively charged hole than to the neutral e^-h^+ complex. (This assumption has been used without any discussion, for example, by Adamowski *et al* (1972).)

For a mathematical proof we present lower bounds to the ground-state energy $E_1^3(\sigma)$ of the $e^-e^-h^+$ complex described by the Hamiltonian

$$H^3(\sigma) = -(\Delta_1+\Delta_2+\sigma\Delta_3)/(1+\sigma)+2/r_{12}-2/r_{13}-2/r_{23}, \tag{31}$$

which lie above the ground-state energy of two free excitons (i.e. above -2). We estimate rather crudely

$$E_1^3(\sigma) \geq E_1(H^3(\sigma)+\sigma\Delta_3/(1+\sigma)) = (1+\sigma)E_1(H_{H^-}). \tag{32}$$

Since Grosse *et al* (1978) have found a lower bound of -1.0834 to the ground-state energy of the H^- ion, for $\sigma \leq 0.84$ we can continue (32) in the following way:

$$(1+\sigma)E_1(H_{H^-}) > -(1+\sigma)\times 1.0834 > -2. \tag{33}$$

Using $E_1(H_{H_2^+}) > -1.208$ (Grosse *et al* 1978) we analogously conclude for $\sigma \geq 1.53$

$$E_1^3(\sigma) \geq E_1(H^3(\sigma)+(\Delta_1+\Delta_2)/(1+\sigma)) = [(1+\sigma)/\sigma]E_1(H_{H_2^+}) > -2. \tag{34}$$

For $0.84 < \sigma \leq 1$ we estimate

$$E_1^3(\sigma) \geq E_1(H^3(\sigma)+(1-\sigma)(\Delta_1+\Delta_2)/(1+\sigma)) = (1+\sigma)E_1(H_{e^+e^-e^-})/\sigma \tag{35}$$

and for $1 < \sigma < 1.53$

$$E_1^3(\sigma) \geq E_1(H^3(\sigma)+(\sigma-1)\Delta_3/(1+\sigma)) = (1+\sigma)E_1(H_{e^+e^-e^-}). \tag{36}$$

To ensure that the right-hand sides of (35) and (36) are greater than -2, we only need $E_1(H_{e^+e^-e^-}) > -0.790$. This doubtless can be proven by the projection method (cf e.g. Thirring 1979, § 3.5, 31) since a variational calculation of high accuracy (Kolos *et al* 1960) yields $E_1(H_{e^+e^-e^-}) = -0.524$. Thus we have shown that the ground-state energy of the $e^+e^-e^-$ complex lies for all σ above that of two free excitons. Therefore, due to the HVZ-theorem (cf e.g. Reed and Simon 1978, theorem 13.17), the essential spectrum of the biexciton begins at -2 which proves, in combination with (30), the stability of the biexciton.

Remark 20. Adamowski *et al* (1972) conclude the stability, monotonicity and concavity of $E_1(\sigma)$ from the examination of the first two derivatives of $E_1(\sigma)$ with respect to σ. But the statement (between relations (2) and (3) in their paper) that an eigenvalue of the Hamiltonian (23) is analytic was not proved in their appendix. In the case of degeneracy the left and right derivatives exist but in general they do not coincide. Therefore the eigenvalues need not be analytic in the points with degeneracy. Concerning the *first* eigenvalue, one can conclude the analyticity with the help of theorems 12.8 and 13.46 in Reed and Simon (1978). Then theorem 19 yields $dE_1(\sigma)/d\sigma \geq 0$ and $d^2E_1(\sigma)/d\sigma^2 \leq 0$ for $\sigma \in [0; 1]$: $dE_1(\sigma)/d\sigma \leq 0$ for $\sigma \in [1; \infty)$.

Putting $\sigma_1 = 0$ and $\sigma_2 = 1$ into (28) we see that for the binding energy $E_B(\sigma) = E_1(\sigma)+2$ it holds that

$$E_B(\sigma) \geq (E_B(0)/2+\sigma(E_B(1)-E_B(0))/(1+\sigma))2 \tag{37}$$

i.e. the binding energy lies above a concave hyperbola going through the points $(0; E_B(0))$ and $(1; E_B(1))$. Adamowski *et al* (1972) only obtained that $E_B(\sigma)$ lies above the straight line through $(0; E_B(0))$ and $(1; E_B(1))$:

$$E_B(\sigma) \geq (1-\sigma)E_B(0)+\sigma E_B(1). \tag{38}$$

Obviously (38) is a conclusion from the concavity condition $d^2E_1(\sigma)/d\sigma^2 \leq 0$. Our inequality (37) is related to the sharper estimation

$$d^2E_1(\sigma)/d\sigma^2 \leq -(2/(1+\sigma))\, dE_1(\sigma)/d\sigma \tag{39}$$

which follows, like (28), from the concavity of $E_1(\alpha)$:

$$0 \geq d^2\bar{E}_1(\alpha)/d\alpha^2 = (d\sigma/d\alpha)^2\, d^2E_1(\sigma)/d\sigma^2 + (d^2\sigma/d\alpha^2)\, dE_1(\sigma)/d\sigma$$
$$= (1+\sigma)^4(d^2E_1(\sigma)/d\sigma^2 + (2/(1+\sigma))\, dE_1(\sigma)/d\sigma).$$

Already the weaker version of our theorem 19 by Adamowski *et al* (1972) suffices to reject the calculation by Sharma (1968b) as it yields a qualitatively wrong behaviour of the energy with respect to σ. Our qualitative statements of § 3 reject the Coulomb approximation for the system $D^+ + A^- +$exciton (cf remark 14). These are examples of the value of rigorous, qualitative statements.

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Note added in proof. Due to § 5 in Alvarez-Estrado and Galindo (1978) a finer classification of theorem 8(b) is possible: If the sum of the charges of the heavy particles ΣZ_k is zero or has the same sign as the light particles then $\alpha_i > 0$. If the sign of ΣZ_k is opposite to that of the light particles then $\alpha_i = 0$ for every i.

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