EXPECTATION VALUES OF QUASIBOUND STATES: NUCLEAR QUADRUPOLE COUPLING CONSTANTS OF BH IN THE $\tilde{X}^1\Sigma^+$ AND $\tilde{B}^1\Sigma^+$ STATES

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The ^{10}B and ^{11}B nuclear quadrupole coupling constants of the bound and quasibound rotation-vibrational levels of BH in the ground $\tilde{X}^1\Sigma^+$ and double-minimum excited $\tilde{B}^1\Sigma^+$ electronic states are evaluated using *ab initio* calculated potentials and electric field gradients. The predicted expectation values of the resonance states are found to be smooth continuations of those of the bound states, but their dependence on the rotational and vibrational quantum numbers differs from the standard Dunham-type polynomial dependences obtained for bound state constants.

Key words: Expectation values; ^{10}B and ^{11}B Nuclear quadrupole coupling constants; Resonance states; Boron; *Ab initio* calculations.

Highly excited rotation-vibrational bound and quasibound resonance or metastable states have a strong influence on the molecular internal state distributions and the reaction characteristics[1]. Theoretically they have been described for a broad variety of systems[2] and their importance for scattering phenomena is well established. Their direct experimental detection in scattering experiments is a difficult and still unsolved task[3] due to the insufficient energy resolution of the experimental setups used for this purpose. Applying however high-resolution spectroscopic methods accurate energy measurements of metastable states became recently possible especially in cases where the reseonances have a long lifetime[4–6]. Metastable states, especially those which act as "transition states" of reaction complexes, are crucially important in quantum mechanical formulations of reaction dynamics. Their experimental and theoretical verification is a challenging new field in modern molecular science.

The positions and wavefunctions of low-lying resonances were previously shown to be very sensitive to small changes of the asymptotic form of the potential energy surfaces[7]. The same sensitivity can also be observed for the electric dipole transitions from

metastable to bound states and for theoretical rate determinations of low-temperature radiative association reactions. The effect on the other hand of the transitions from bound to quasibound states on the mean internuclear separation of a diatomic model system was recently found to be less significant[8]. Systematic studies of the behaviour of the expectation values of molecular properties of quasibound states are rather sparse. In the simple case of one-dimensional systems reliable calculations can be conveniently done making use of the Pajunen's approach[8] based on Rayleigh–Schrodinger perturbation theory formulated in terms of the complex Prufer phase function. For more-dimensional problems this approach is not suitable and other alternative schemes have to be adopted as for example the complex scaling method discussed recently[9].

An especially simple procedure can be applied when dealing with molecular properties causing only small perturbations of the rotation-vibrational levels such as for example in the fine and hyperfine splittings of spectral lines. In such a case, all degrees of freedom except for rotational and vibrational motions can be integrated over and using suitable basis sets the resulting diagonal elements of the perturbation matrix can be absorbed into the total potential energy function. The energy positions of the perturbed quasibound states are then calculated using practically the same methods which are usually applied for evaluating energies and lifetimes of the unperturbed states[10–13].

In the present study the performance of the proposed procedure is tested evaluating the expectation values of the nuclear quadrupole coupling constants of the BH molecule. The actual calculations are done for the $^{10}B^1H$ and $^{11}B^1H$ isotopic species in their ground $\tilde{X}^1\Sigma^+$ and double-minimum excited $\tilde{B}^1\Sigma^+$ electronic states for which complete sets of accurate *ab initio* potential energy and electric field gradient data are available from the literature[14–19]. The nuclear quadrupole coupling is a simple potential-like perturbation which can be exactly accounted for by incorporating it into the associated rotation-vibrational Schrödinger equations[20] and the corresponding nuclear coupling splittings are expected to exhibit a strong vibrational dependence[21]. In addition, due to the fairly large nuclear quadrupole moments of the boron isotopes the resulting splittings of the spectra are most probably detectable especially when applying microwave spectroscopy techniques recently developed by Carrington and his coworkers[6].

THEORETICAL

Effective Hamiltonians

In this study we restrict ourselves to the case of well isolated electronic states of diatomic molecules possesing only one nucleus with nonzero quadrupole moment. In this case, the Hamiltonian describing interaction between a nuclear quadrupole moment and molecular electric fields may be expressed in the following form[20]

$$\hat{H}^{\mathrm{iAIJF}}_{\mathrm{NQ}}(R) = -eQ_{\mathrm{A}}\, q_m^{\mathrm{iA}}(R)\, f(I,J,F) \ , \qquad (1)$$

where Q_{A} is effective nuclear quadrupole moment of the "quadrupole active" nucleus A, R is the separation of the nucleus A from the other nucleus (possesing no quadrupole moment), $q_m^{\mathrm{iA}}(R)$ is the zz component of the electric field gradient (EFG) tensor at the nucleus A taken along the direction of the molecular axis, F is the quantum number of the total angular momentum, $\hat{F} = \hat{I} + \hat{J}$ ($\hat{I}$ and $\hat{J}$ being the nuclear spin and angular momentum caused by molecular rotation), and $f(I,J,F)$ is Casimir's function

$$f(I, J, F) = \frac{\frac{3}{4}C(C+1) - I(I+1)\, J(J+1)}{2I(2I-1)\,(2J-1)\,(2J+3)}$$

$$C = F(F+1) - I(I+1) - J(J+1) \ . \qquad (2)$$

The function $q_m^{\mathrm{iA}}(R)$, pertaining to a given electronic molecular state i, can easily be evaluated using the corresponding Born–Oppenheimer wavefunction $\Psi_i(\bar{\boldsymbol{r}}_k;R)$

$$q_m^{\mathrm{iA}}(R) = eZ_n \frac{2}{R^3} - e\, \langle \Psi_i(\bar{\boldsymbol{r}}_k;\, R) \left| \sum_k \frac{3z_{k\mathrm{A}}^2 - r_{k\mathrm{A}}^2}{r_{k\mathrm{A}}^5} \right| \Psi_i(\bar{\boldsymbol{r}}_k;\, R) \rangle_{\bar{r}_k} \ , \qquad (3)$$

where Z_n is the atomic number of the other nucleus and coordinates are chosen with nucleus A at the origin.

The unperturbed ro-vibrational energies, E, and wavefunctions, $\chi(R)$, pertaining to the given electronic state can be obtained as solutions of the following Schrodinger equation

$$\frac{\mathrm{d}^2}{\mathrm{d}R^2}\chi(R) + \frac{2\mu}{\hbar^2}\left[E - V_i(R) - \frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2}\right]\chi(R) = 0 \qquad (4)$$

with

$$\chi(R) \equiv \chi_{vJ}(R) \quad \text{for} \ E_{vJ} < 0$$

$$\equiv \chi_{kJ}(R) \quad \text{for} \ E > 0 \ , \ E = (\hbar^2 k^2)/(2\mu) \ . \qquad (5)$$

The wavefunctions are normalized such that for the bound states ($E < 0$) $\int \chi_{vJ}^2(R)\, dR = 1$ and for the continuum states with positive energies the functions $\chi_{kJ}(R)$ are assumed to approach an asymptotic sinoidal form according to

$$\lim_{R\to\infty} = \sin\,(kR - \pi J/2 + \delta_J) \tag{6}$$

with δ_J describing the phase shift of J-th partial wave.

The nuclear quadrupole coupling term can nearly always be treated as a small perturbation of the ro-vibrational Hamiltonian. Thus, the corresponding energy splittings of the bound ro-vibrational states can be approximated (fairly quantitatively) by means of the first-order perturbation theory

$$\Delta E^{(1)}_{i\mathrm{A}vIJF} = \langle \chi_{vJ}(R)\, |\hat{H}^{i\mathrm{A}IJF}_{NQ}|\, \chi_{vJ}(R)\rangle_R \; =$$

$$= -eQ_{\mathrm{A}}\, f(I,J,F)\, \langle \chi_{vJ}(R)\, |q^{i\mathrm{A}}_m(R)|\, \chi_{vJ}(R)\, \rangle_R \;, \tag{7}$$

where the quantities

$$(\mathrm{NQCC})_{i\mathrm{A}vJ} = eQ_{\mathrm{A}}\, \langle v, J\, |q^{i\mathrm{A}}_m(R)|\, v, J\rangle_R \tag{8}$$

provides theoretical rationalization of the so-called nuclear quadrupole coupling constants (NQCC) which are usually derived from experimental spectra. The "exact" values of the nuclear quadrupole energies, E_{vIJF}, are obtainable as the eigenvalues of the radial Schrodinger equation (*4*) with the following effective potential

$$V_i(R) + \frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2} - eQ_{\mathrm{A}}\, q^{i\mathrm{A}}_m(R)\, f(I,J,F) \;. \tag{9}$$

Theoretical rationalization of the nuclear quadrupole splittings in the resonance states is less straightforward. The problem stems from the fact that the resonance wavefunctions are not square integrable and cannot be thus used for the standard evaluation of the expectation values like that one given by Eq. (*8*). To solve this problem one can use either appropriate convergence factors (which is *de facto* equivalent to using the complex scaling method; for more details and references see ref.[9]) or analytic continuation which allows evaluation of the expectation values of the resonance states by means of the continuum states having energies close to the resonance energies[22]. Quite generally, however, the resulting, mathematically correct, expectation values are complex num-

bers (this seems to cast some doubts on the formal mathematical correctness of the definition of the expectation value in ref.[8]).

Though it makes sense, and is also fairly feasible, dealing with complex nuclear quadrupole constants (or any other spectroscopic constants) is rather inconvenient. This leads us to abandon their usual rationalization *via* the expectation values of the electric field gradient $q_m^{iA}(R)$ and replace it by a more "orthodox" definition. This definition is based on the fact that the "exact" evaluation of the nuclear quadrupole splittings is legitimate not only for the bound states, but also for all the continuum states, particularly for the long-living resonance states which can be probed spectroscopically. Once the resonance states are localized with the use of any of the above-mentioned techniques[10–13] (let us adopt the common convention and label them $|v,J\rangle$ as a continuation of bound states into the continuum region), we can repeatedly solve the radial Schrödinger equation with the perturbed potential (*9*) and obtain the quadrupole splittings in the same way as for the bound states. Using Eq. (*7*), obviously, the splittings can be used to evaluate the sought effective and real nuclear quadrupole constants for the studied resonance states $\langle \chi_{kJ}(R) \, |q_m^{iA}(R)| \, \chi_{kJ}(R) \rangle_{\text{eff}}$.

Computational Details

The electric field gradient (EFG) data for the $\tilde{X}^1\Sigma^+$ and $\tilde{B}^1\Sigma^+$ states of boron hydride are taken from the literature[14,16]. The data points are interpolated using cubic splines whereas extrapolation to their asymptotic values is done assuming a $aR^{-6} + bR^{-8}$ dependence. Potential energies for the $\tilde{X}^1\Sigma^+$ state[18] and the $\tilde{B}^1\Sigma^+$ state potential which are merged from the data in refs[16,19] are summarized in Table I. Nuclear quadrupole mo-

TABLE I
Potential energy curve of the $\tilde{B}^1\Sigma^+$ state of BH molecule

R, a.u.	*E*, cm^{-1}	*R*, a.u.	*E*, cm^{-1}	*R*, a.u.	*E*, cm^{-1}
1.20	79 373.3	3.25	–9 786.0	8.00	–7 058.0
1.40	32 181.9	3.50	–8 300.2	9.00	–4 670.1
1.60	6 025.3	3.75	–7 659.3	10.00	–2 855.0
1.90	–11 634.0	4.00	–7.828.3	12.00	–615.7
2.00	–14 302.8	4.25	–8 844.5	15.00	–57.6
2.10	–15 911.6	4.50	–10 001.1	18.00	–11.5
2.30	–17 070.4	5.00	–11 653.8	21.00	–4.5
2.50	–16 491.0	5.50	–12 378.0	25.00	–1.6
2.75	–14 526.7	6.00	–12 066.4		
3.00	–12 051.0	7.00	–9 832.1		

TABLE II
Vibrational dependences of the boron NQCCs in the $\tilde{X}^1\Sigma^+$ electronic state of ^{10}BH for selected rotational states (B bound, Q quasibound)

v	NQCC, MHz				
	J = 10	*J* = 20	*J* = 30	*J* = 40	*J* = 50
0	–13.594 B	–13.161 B	–12.475 B	–11.571 B	–10.514 B
1	–13.236 B	–12.817 B	–12.147 B	–11.278 B	–10.288 B
2	–12.883 B	–12.480 B	–11.840 B	–11.016 B	–10.087 B
3	–12.544 B	–12.162 B	–11.557 B	–10.765 B	–9.946 B
4	–12.228 B	–11.865 B	–11.281 B	–10.559 B	–9.843 Q
5	–11.927 B	–11.577 B	–11.038 B	–10.389 B	–9.794 Q
6	–11.640 B	–11.317 B	–10.828 B	–10.250 B	–9.847 Q
7	–11.384 B	–11.089 B	–10.649 B	–10.148 B	–10.286 Q
8	–11.157 B	–10.891 B	–10.497 B	–10.099 B	
9	–10.960 B	–10.719 B	–10.379 B	–10.120 Q	
10	–10.789 B	–10.576 B	–10.305 B	–10.258 Q	
11	–10.645 B	–10.469 B	–10.282 B	–10.626 Q	
12	–10.536 B	–10.404 B	–10.326 B		
13	–10.467 B	–10.386 B	–10.463 Q		
14	–10.442 B	–10.428 B	–10.706 Q		
15	–10.468 B	–10.542 B			
16	–10 557 B	–10.728 B			
17	–10.707 B	–11.005 Q			
18	–10.909 B				
19	–11.272 B				

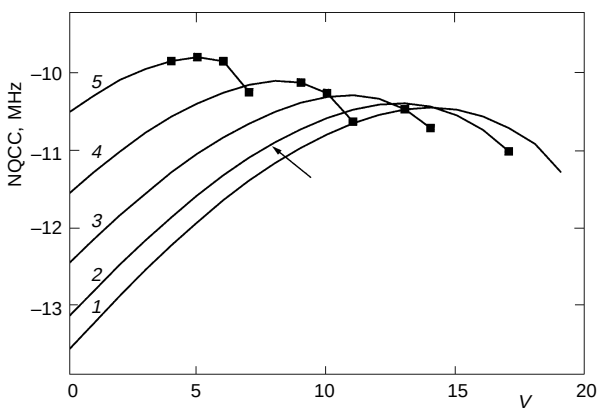

FIG. 1
Vibrational dependences of the boron NQCCs in the $X^1\Sigma^+$ electronic state of ^{10}BH. Squares denote quasibound states; *J* = 10 (*1*), 20 (*2*), 30 (*3*), 40 (*4*), 50 (*5*)

TABLE III
Vibrational dependences of the boron NQCCs in the $\tilde{X}^1\Sigma^+$ electronic state of ^{11}BH for selected rotational states (B bound, Q quasibound)

v	NQCC, MHz				
	J = 10	*J* = 20	*J* = 30	*J* = 40	*J* = 50
0	–6.523 B	–6.318 B	–5.991 B	–5.560 B	–5.056 B
1	–6.353 B	–6.153 B	–5.834 B	–5.420 B	–4.947 B
2	–6.184 B	–5.992 B	–5.687 B	–5.294 B	–4.850 B
3	–6.021 B	–5.840 B	–5.551 B	–5.173 B	–4.781 B
4	–5.870 B	–5.698 B	–5.419 B	–5.074 B	–4.730 Q
5	–5.726 B	–5.560 B	–5.302 B	–4.992 B	–4.704 Q
6	–5.589 B	–5.435 B	–5.201 B	–4.924 B	–4.722 Q
7	–5.466 B	–5.325 B	–5.115 B	–4.874 B	–4.881 Q
8	–5.357 B	–5.230 B	–5.042 B	–4.848 B	
9	–5.263 B	–5.147 B	–4.984 B	–4.855 Q	
10	–5.180 B	–5.078 B	–4.947 B	–4.914 Q	
11	–5.111 B	–5.026 B	–4.934 B	–5.072 Q	
12	–5.058 B	–4.994 B	–4.952 B		
13	–5.024 B	–4.983 B	–5.013 B		
14	–5.010 B	–5.001 B	–5.124 Q		
15	–5.021 B	–5.053 B			
16	–5.062 B	–5.139 B			
17	–5.131 B	–5.264 Q			
18	–5.226 B				
19	–5.385 B				

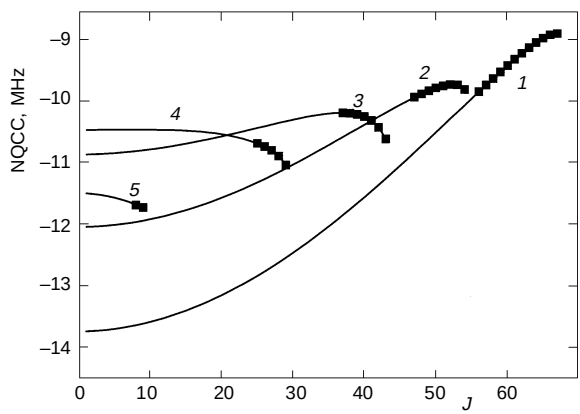

FIG. 2
Rotational dependences of the boron NQCCs in the $X^1\Sigma^+$ electronic state of ^{10}BH. Squares denote quasibound states; *v* = 0 (*1*), 5 (*2*), 10 (*3*), 15 (*4*), 20 (*5*)

ment values of 0.08472 and 0.04065 barns are used for the ^{10}B and ^{11}B isotopes, respectively.

The radial Schrodinger equations are solved numerically applying the standard Numerov–Cooley finite difference procedure[23] with 8 000 integration points uniformly distributed in the range from 0 to 70 a.u. This ensures a high accuracy of the integration scheme and a safe convergence behaviour for all the calculated resonance states of both isotopomers. The resonances are localized using the internal amplitude criterion ap-

TABLE IV
Rotational dependences of the boron NQCCs in the $\tilde{X}^1\Sigma^+$ electronic state of ^{10}BH for selected vibrational states (B bound, Q quasibound)

J	NQCC, MHz				
	v = 0	*v* = 5	*v* = 10	*v* = 15	*v* = 20
0	–13.749 B	–12.053 B	–10.871 B	–10.469 B	–11.500 B
3	–13.732 B	–12.039 B	–10.862 B	–10.469 B	–11.531 B
6	–13.690 B	–12.005 B	–10.839 B	–10.468 B	–11.607 B
9	–13.622 B	–11.950 B	–10.803 B	–10.468 B	–11.754 Q
12	–13.529 B	–11.874 B	–10.755 B	–10.472 B	
15	–13.411 B	–11.779 B	–10.696 B	–10.485 B	
18	–13.269 B	–11.664 B	–10.627 B	–10.512 B	
21	–13.104 B	–11.530 B	–10.550 B	–10.563 B	
24	–12.915 B	–11.380 B	–10.468 B	–10.651 B	
27	–12.706 B	–11.215 B	–10.384 B	–10.805 Q	
30	–12.475 B	–11.038 B	–10.305 B		
33	–12.225 B	–10.850 B	–10.237 B		
36	–11.956 B	–10.654 B	–10.197 B		
39	–11.670 B	–10.455 B	–10.221 Q		
42	–11.369 B	–10.257 B	–10.432 Q		
45	–11.055 B	–10.064 B			
48	–10.732 B	–9.888 Q			
51	–10.404 B	–9.759 Q			
54	–10.074 B	–9.820 Q			
57	–9.746 Q				
60	–9.428 Q				
63	–9.139 Q				
66	–8.932 Q				

proach[10] which gives also directly halfwidths and the Airy function localization scheme including a semiclassical halfwidth calculation[11]. Both approaches provided practically identical energy positions and the halfwidths differ by not more than 1–2 per cent in the medium range of their values.

RESULTS AND DISCUSSION

The calculations of the boron nuclear coupling constants (NQCC) are performed for all the spectroscopically relevant bound and quasibound rotation-vibrational states of the

TABLE V
Rotational dependences of the boron NQCCs in the $\tilde{X}^1\Sigma^+$ electronic state of ^{11}BH for selected vibrational states (B bound, Q quasibound)

J	NQCC, MHz				
	v = 0	*v* = 5	*v* = 10	*v* = 15	*v* = 20
0	–6.598 B	–5.786 B	–5.220 B	–5.023 B	–5.499 B
3	–6.589 B	–5.780 B	–5.215 B	–5.022 B	–5.515 B
6	–6.569 B	–5.764 B	–5.204 B	–5.021 B	–5.553 B
9	–6.537 B	–5.737 B	–5.187 B	–5.021 B	–5.627 Q
12	–6.493 B	–5.701 B	–5.164 B	–5.022 B	
15	–6.436 B	–5.656 B	–5.136 B	–5.028 B	
18	–6.369 B	–5.601 B	–5.103 B	–5.040 B	
21	–6.290 B	–5.538 B	–5.066 B	–5.062 B	
24	–6.201 B	–5.466 B	–5.026 B	–5.102 B	
27	–6.101 B	–5.387 B	–4.986 B	–5.171 Q	
30	–5.991 B	–5.302 B	–4.947 B		
33	–5.872 B	–5.212 B	–4.914 B		
36	–5.744 B	–5.119 B	–4.892 B		
39	–5.607 B	–5.024 B	–4.899 Q		
42	–5.464 B	–4.928 B	–4.984 Q		
45	–5.314 B	–4.836 B			
48	–5.160 B	–4.750 Q			
51	–5.003 B	–4.686 Q			
54	–4.846 B	–4.692 Q			
57	–4.689 Q				
60	–4.536 Q				
63	–4.396 Q				
66	–4.291 Q				

^{10}BH and ^{11}BH isotopomers in their $\tilde{X}^1\Sigma^+$ and $\tilde{B}^1\Sigma^+$ electronic states. Typical results of these calculations are collected in Tables II–VI and shown in Figs 1–3. To a large extent the ratio NQCC(^{10}BH)/NQCC(^{11}BH) is nearly state independent and is approxi-

TABLE VI
Rotational dependences of the boron NQCCs in the $\tilde{B}^1\Sigma^+$ electronic state of ^{10}BH and ^{11}BH for v = 0 and v = 1 states (B bound, Q quasibound)

J	NQCC, MHz			
	^{10}BH		^{11}BH	
	v = 0	v = 1	v = 0	v = 1
2	–10.242 B	–10.002 B	–4.915 B	–4.800 B
4	–10.231 B	–9.989 B	–4.910 B	–4.794 B
6	–10.215 B	–9.969 B	–4.902 B	–4.784 B
8	–10.192 B	–9.941 B	–4.891 B	–4.771 B
10	–10.163 B	–9.905 B	–4.877 B	–4.754 B
12	–10.127 B	–9.861 B	–4.860 B	–4.733 B
14	–10.085 B	–1.756 B	–4.840 B	–0.843 B
16	–10.037 B	–1.742 B	–4.817 B	–0.836 B
17	–10.010 B	–1.735 B	–4.804 B	–0.833 B
18	–9.982 B	–1.727 B	–4.791 B	–0.829 B
19	–9.952 B	–1.718 B	–4.776 B	–0.825 B
20	–1.710 B	–9.920 B	–0.821 B	–4.761 B
21	–1.700 B	–9.886 B	–0.816 B	–4.745 B
22	–1.691 B	–1.618 B	–0.812 B	–0.777 B
23	–1.681 B	–1.607 B	–0.807 B	–0.772 B
24	–1.670 B	–1.596 B	–0.802 B	–0.766 B
25	–1.659 B	–1.584 B	–0.797 B	–0.761 B
30	–1.599 B	–1.521 B	–0.768 B	–0.731 B
40	–1.451 B	–1.369 B	–0.698 B	–0.658 B
50	–1.269 B	–1.191 B	–0.611 B	–0.574 B
60	–1.056 B	–0.995 B	–0.510 B	–0.480 B
70	–0.825 B	–0.788 B	–0.399 B	–0.381 B
80	–0.595 B	–0.580 B	–0.289 B	–0.282 B
85	–0.489 Q	–0.479 Q	–0.238 Q	–0.233 Q
90	–0.392 Q	–0.382 Q	–0.191 Q	–0.187 Q
95	–0.306 Q	–0.289 Q	–0.150 Q	–0.142 Q
100	–0.229 Q	–0.204 Q	–0.113 Q	–0.101 Q
105	–0.152 Q	–0.125 Q	–0.076 Q	–0.064 Q

mately equal to the ratio of the ^{10}B and ^{11}B nuclear quadrupole moments. The figures therefore provide an illustration for the both isotopomers.

In Fig. 1 and also in Tables II and III typical vibrational dependences of the calculated NQCCs are described. The "parabolic" shape of these dependences is very similar to the shape of the pertinent EFG and with increasing delocalization of the molecular wavefunctions towards the asymptotic region. The NQCCs of the resonance states appear as smooth continuations of the bound state constants. The dependences of the NQCCs on the rotational quantum numbers shown in Fig. 2 and summarized in Tables IV and V are more complicated compared to the pure vibrational states. Nevertheless, the NQCCs of the resonances can again be viewed as smooth continuations of the bound state values.

The excited $\tilde{B}^1\Sigma^+$ state of boron hydride has a double-minimum potential forcing all the low-lying bound states to be located in one of the potential wells. This leads to a rather peculiar stepwise behaviour of the dependences of the calculated NQCCs on the rotation-vibrational quantum numbers such as described previously[15]. The resonance states are totally unaffected by the double-minimum character of the potential because the potential barrier is much below the energy of the dissociation limit. Therefore, like in the case of a single-minimum potential, the calculated NQCC values are obtained as smooth continuations of their bound state counterparts (Fig. 3 and Table VI).

CONCLUSIONS

Model calculations are performed in the present study to test the applicability of the standard first-order perturbation theory approach used for evaluating expectation values

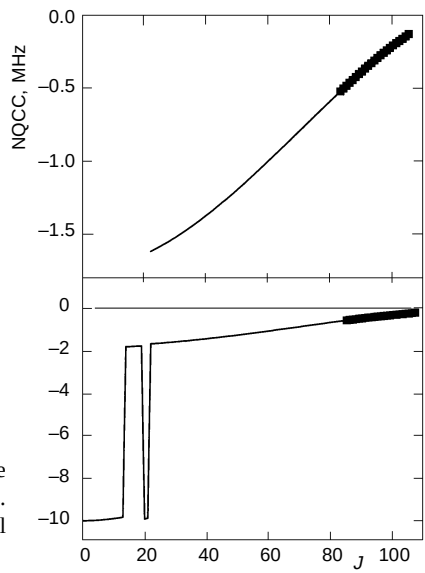

FIG. 3
Rotational dependence of the boron NQCCs in the $B^1\Sigma^+$ electronic state of ^{10}BH for $v = 1$ states. Squares denote quasibound states; the upper panel is a magnification of the lower one

of bound state properties in one-dimensional systems also to quasibound state properties. For this purpose the ^{10}B and ^{11}B nuclear quadrupole coupling constants of the bound and quasibound rotation-vibrational states of boron hydride in the ground $\tilde{X}^1\Sigma^+$ and the double-minimum excited $\tilde{B}^1\Sigma^+$ states are evaluated from *ab initio* calculated potential energies and electric field gradients. It is shown here that the NQCC values obtained for the quasibound states are smooth continuations of their bound state counterparts. The dependence of the quasibound states constants on the rotation-vibrational quantum numbers however is different from the situation for the bound state levels. This means that they cannot be obtained by simple extrapolations from the bound states values, but only by explicit calculations such as performed in the present study.

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