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Spectral properties of a short-range impurity in a quantum dot

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The spectral properties of the quantum mechanical system consisting of a quantum dot with a short-range attractive impurity inside the dot are studied in the zero-range limit. The Green function of the system is obtained in an explicit form. In the case of a spherically symmetric quantum dot, the dependence of the spectrum on the impurity position and strength of the impurity potential is analyzed in detail. The recovering of the confinement potential of the dot from the spectroscopy data is proven; the consequences of the hidden symmetry breaking by the impurity are considered. The effect of the positional disorder is analyzed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1647693]

I. INTRODUCTION

Quantum dots (i.e., nanostructures with charge carriers confinement in all spatial directions) have an atom-like energy spectrum and, therefore, make possible to fabricate quantum devices with energy level spacing much greater than the temperature smearing kT at work temperature T (see, e.g., Ref. 1). Moreover, dimension and shape of a quantum dot affect considerably the most important characteristics of the corresponding devices: Relaxation and recombination time, Auger recombination coefficient etc, thus a possibility arises to control such characteristics in manufacturing the devices.[2–4] Another way to control the properties of a quantum dot is instilling an impurity into the dot. Therefore, the investigation of spectral properties of a quantum dot with impurities as well as the dependence of the spectrum on the geometric parameters of the dot and physical characteristics of the impurity is an important problem of nano- and mesoscopic physics (see, e.g., in Refs. 5–7, and references therein). The case of a hydrogen-like impurity is one of the most extensively studied up to now; however, the spectral problem in this case has no exact solution. On the other hand, short-range impurities can be investigated in the framework of the point potential theory (also called the zero-range potential theory). An important peculiarity of the point potential method is that the spectral problem for a point perturbed Hamiltonian is explicitly soluble as soon as the Green function for the unperturbed operator is known in an explicit form.[8,9]

For modeling the geometric confinement of a quantum dot, quadratic (in other words, parabolic) potentials are successfully used[10] (see also examples of applications in Refs. 5–7, 11–15). The reason is that the self-consistent solution to the corresponding system of the Poisson and Schrödinger equations leads to the confinement potential having the form of a truncated parabolic potential.[16] Moreover, the Green function of the corresponding Hamiltonian $\hat{H}^0$,

$$\hat{H}^0 = -\frac{\hbar^2}{2\mu}\Delta + \frac{\mu\Omega^2}{2}r^2, \tag{1}$$

can be explicitly calculated[17–19] (here Ω is the frequency of the oscillator, μ denotes over the

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paper the mass of the considered charged particle). This makes possible to perform an exhaustive spectral analysis of the perturbation of $\hat{H}^0$ by a point potential of arbitrary position $\mathbf{q}$ and strength α [we denote this perturbation by $\hat{H}_\alpha(\mathbf{q})$] and to analyze the behavior of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$ as functions of $\mathbf{q}$ and α. This analysis is the main goal of the paper. Note that a quite particular case of the point perturbation of $\hat{H}^0$ at $\mathbf{q}=0$ (without obtaining any explicit form for the Green function) has been considered in Ref. 20. Point potential for modeling an impurity in a spherically symmetric quantum dot has been studied in the series of papers using the Green function representation by means of the Laplace transform of the propagator kernel, but this approach allows to analyze (with numerical methods) the lowest impurity level only.[6,13–15]

It should be noted that point perturbations of the one-dimensional harmonic oscillators have been studied in detail earlier. This study was started in Ref. 21, where the spectral properties of the point perturbed harmonic oscillator have been considered in the context of the one-dimensional models for the toponium physics and the Bose–Einstein condensation.[22] A strict mathematical justification of results from Ref. 21 was done in Refs. 23 and 24; see also in Ref. 25. Undoubtedly, our approach using the three-dimensional harmonic oscillator is more adequate for the analyzing the spectral properties of three-dimensional systems, in particular, the toponium. It should be noted also that the one-dimensional harmonic oscillator perturbed by a point potential with varying position and strength has been investigated in Refs. 26 and 27. A series of phenomena of low-dimensional condensed matter physics can be analyzed by means of the Hamiltonian of the perturbed oscillator: Impurity in a one-dimensional quantum well, one-dimensional channel in a two-dimensional heterostructure subjected to a perpendicular uniform magnetic field etc., see the bibliography in the cited papers for details. However, the analysis given in Refs. 26, and 27 is based on the properties of one-dimensional second-order differential operators and is not extended to the three-dimensional case.

The paper is organized as follows. Preliminary results are collected in Sec. II. In Sec. III we consider point perturbations of the operator

$$\hat{H}^0 = -\frac{\hbar^2}{2\mu}\Delta + V, \tag{2}$$

with an infinitely growing potential V. It turns out that the operator $\hat{H}_\alpha(\mathbf{q})$ can be defined and investigated for the more generic case when $\hat{H}^0$ is defined by Eq. (2). In Sec. IV some important properties of $\hat{H}_\alpha(\mathbf{q})$ are established. In particular, a complete description of the spectrum and eigenfunctions of $\hat{H}_\alpha(\mathbf{q})$ is given in Theorem 1. As a consequence of this theorem we get the falling of the considered particle on the attractive center as the potential strength α tends to $-\infty$; for a very particular case of the one-dimensional harmonic oscillator perturbed at the potential minimum this phenomenon was observed in Ref. 21. In Sec. V we define at fixed α a family of continuous functions such that the values of these functions at the point $\mathbf{q}$ form the complete family of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$. Some elementary properties of these functions are established in Theorem 2. The main results of the paper are contained in Sec. VI, where the point perturbations of the Hamiltonian of the harmonic oscillator are studied; the case of the isotropic harmonic oscillator (1) is considered in detail. These results are based on an explicit form of the Green function for the operator (1). The detailed analysis of the dependence of the point levels on the position $\mathbf{q}$ and on the strength α is given in Theorem 3. In particular, if $\mathbf{q}\neq 0$, then the point levels never coincide with the eigenvalues of the unperturbed operator $\hat{H}^0$. Therefore, we have here no accidental degeneracy of the levels, which is a peculiarity of the one-dimensional model for the toponium.[21,26] Hence, this degeneracy is an artifact of the one-dimensional model. Another interesting result is the asymptotic expression for the bound state of $\hat{H}_\alpha(\mathbf{q})$ [Eqs. (33), and (34)]. These equations show that at least for the isotropic harmonic oscillator its potential (i.e., the frequency Ω) can be recovered from the dependence of the ground state of the point perturbation on the support of the perturbation. Moreover, we argue that the form of the parabolic potential V may be recovered from the behavior of the excited energy for the ground state. Our conjecture is that this property is true for a more general form of the potential V. In this connection it is of interest to note that the study of the excited energy is one of the main problems of the quantum dot physics.[6] The methods of Sec. VI allow us to analyze rigorously the phenomenon of so-called ''positional disorder'' in quantum dots (including nonisotropic ones). The relation of the degeneracy properties of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$ at $\mathbf{q}=0$ to the symmetry properties of the unperturbed operator $\hat{H}^0$ in the phase space is briefly discussed in the conclusion of Sec. VI. In particular, the appearance of states with nonzero dipole momentum is noted.

II. PRELIMINARIES

Here we present for the convenience of readers some basic properties of point perturbations of Schrödinger operators in $L^2(\mathbb{R}^3)$ (see, e.g., Refs. 8, 28–31 for details). We will consider only Schrödinger operators $\hat{H}^0$ of the form (2), where the potential V is subordinated to the conditions

(P1) $V\in L^p_{\mathrm{loc}}(\mathbb{R}^3)$ *for some* $p>3$;
(P2) $V_-=\min(V,0)\in L^2(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$.

Conditions (P1), (P2) are weaker than commonly used in applications conditions $V\in L^\infty_{\mathrm{loc}}(\mathbb{R}^3)$ and $V\geqslant c$ with $c\in\mathbb{R}$ but making use of (P1), (P2) requires no change in proving of main results below. It is well known that under these conditions $\hat{H}^0$ is semibounded from below and essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ (see in Ref. 32 Theorem X.28). Further we put, as a rule, $\hbar=1$, $\mu=1/2$ and denote the obtained operator $-\Delta+V$ by H^0. For the domain $\mathcal{D}(H^0)$ of H^0 we have $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)\subset C(\mathbb{R}^3)$. This inclusion implies that the Green function $G^0(\mathbf{x},\mathbf{y};\zeta)$ for H^0 (the integral kernel of the resolvent $R(\zeta)=(H^0-\zeta)^{-1}$) is a Carleman operator, this means that

$$\int_{\mathbb{R}^3}|G^0(\mathbf{x},\mathbf{y};\zeta)|^2\,d\mathbf{y}<+\infty\quad\text{for a.e. }\ \mathbf{x}\in\mathbb{R}^3. \tag{3}$$

Moreover, according to Theorem B.7.2 from Ref. 31, for every fixed ζ, $\zeta\in\mathbb{C}\setminus\mathrm{spec}\,(H^0)$, the function G^0 obeys the following properties:

(G1) *For every* $\zeta\in\mathrm{spec}(\mathrm{H}^0)$ *the function* $G^0(\mathbf{x},\mathbf{y};\zeta)$ *is continuous in the domain* $\{(\mathbf{x},\mathbf{y})\in\mathbb{R}^3\times\mathbb{R}^3:\mathbf{x}\neq\mathbf{y}\}$;
(G2) $|G^0(\mathbf{x},\mathbf{y};\zeta)|\leqslant c_2(\zeta)|\mathbf{x}-\mathbf{y}|^{-1}$;
(G3) *if* $|\mathbf{x}-\mathbf{y}|\geqslant d>0$, *then* $|G^0(\mathbf{x},\mathbf{y};\zeta)|\leqslant c_3(d,\delta,\zeta)\exp(-\delta|\mathbf{x}-\mathbf{y}|)$ *for some* $\delta>0$. *Moreover, if* $\mathrm{Re}\,\zeta<\Sigma\equiv\mathrm{infspec}(H^0)$, *then arbitrary* δ *with* $\delta^2/2<\Sigma-\mathrm{Re}\,\zeta$ *is suitable for this estimate.*

From (G1) we get, in particular, that (3) is valid for *every* $\mathbf{x}\in\mathbb{R}^3$.

The crucial role in the point potential theory is played by the regularized Green function

$$G^0_{\mathrm{reg}}(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\mathbf{y};\zeta)-\frac{1}{4\pi}\frac{1}{|\mathbf{x}-\mathbf{y}|}. \tag{4}$$

In the particular cases, e.g., if $V\in C^\infty(\mathbb{R}^3)$, it is known that at fixed ζ this function has a continuous extension on the whole space $\mathbb{R}^3\times\mathbb{R}^3$ (see, e.g., Ref. 33 or Theorem III.5.1 in Ref. 34). We need this property in the general situation and prove it under conditions (P1), (P2).

It is sufficient to prove that $G^0_{\mathrm{reg}}(\mathbf{x},\mathbf{y};\zeta)$ is continuous with respect to $(\mathbf{x},\mathbf{y})$ for some $\zeta=E_0<0$. Indeed, then for every $\zeta\in\mathbb{C}\setminus\mathrm{spec}\,(H^0)$

$$G^0(\mathbf{x},\mathbf{y};\zeta)=\int_{E_0}^{\zeta}\frac{\partial}{\partial\lambda}G^0(\mathbf{x},\mathbf{y};\lambda)\,d\lambda+G^0(\mathbf{x},\mathbf{y};E_0),$$

where the path of integration lies in the resolvent set $\mathbb{C}\setminus\mathrm{spec}\,(H^0)$. The function $(\partial G^0/\partial\lambda)(\mathbf{x},\mathbf{y};\lambda)$ is jointly continuous with respect to $(\mathbf{x},\mathbf{y})$ since it coincides with the integral kernel of $(H^0-\lambda)^{-2}$ and this kernel is continuous according to Theorem B.7.1 from Ref. 31.

It is easy to see that V can be represented in the form $V=V_1+W$, where $V_1\in C^\infty(\mathbb{R}^3)$ and obeys the property (P2) and $W\in L^p(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$. Denote $H^1=-\Delta+V_1$, $\Sigma_1=\mathrm{infspec}\,(H^1)$ and by G^1 the Green function of H^1. Fix E_0, $E_0<\min(\Sigma,\Sigma^1)$, and introduce the function $F(\mathbf{x},\mathbf{y},\mathbf{z})=G^0(\mathbf{x},\mathbf{z};E_0)W(\mathbf{z})G^1(\mathbf{z},\mathbf{y};E_0)$. Using properties (G2), (G3), and the estimate

$$\int_{|\mathbf{y}-\mathbf{a}|\leqslant r}\frac{d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|^{\nu}}\leqslant\tilde{c}_{\nu}r^{3-\nu}, \tag{5}$$

where $0<\nu<3$, $r>0$, $\mathbf{a}$, $\mathbf{x}\in\mathbb{R}^3$, it is easy to prove that $F(\mathbf{x},\mathbf{y},\cdot)\in L^1(\mathbb{R}^3)$ for all $\mathbf{x},\mathbf{y}\in\mathbb{R}^3$. In virtue of the Lippmann–Schwinger relation

$$G^0(\mathbf{x},\mathbf{y};E_0)=G^1(\mathbf{x},\mathbf{y};E_0)+\int_{\mathbb{R}^3}G^0(\mathbf{x},\mathbf{z};E_0)W(\mathbf{z})G^1(\mathbf{z},\mathbf{y};E_0)\,d\mathbf{z},$$

and the continuity of the regularized Green function for H^1, it remains to prove that the function

$$I(\mathbf{x},\mathbf{y})=\int_{\mathbb{R}^3}F(\mathbf{x},\mathbf{y},\mathbf{z})\,d\mathbf{z}$$

is continuous on $\mathbb{R}^3\times\mathbb{R}^3$. Moreover, (G1) shows that it remains to prove the continuity of I at points of the form $(\mathbf{x}_0,\mathbf{x}_0)$. To do this fix $\varepsilon>0$ and find $\eta>0$ such that the relations $|\mathbf{x}-\mathbf{x}_0|<\eta$, $|\mathbf{y}-\mathbf{x}_0|<\eta$ imply $|I(\mathbf{x},\mathbf{y})-I(\mathbf{x}_0,\mathbf{x}_0)|\leqslant\varepsilon$. Introduce the sets $B_1(\eta)=\{\mathbf{z}\colon|\mathbf{z}-\mathbf{x}_0|<\eta\}$, $B_2(\eta)=\mathbb{R}^3\backslash B_1(\eta)$, and for a measurable set $B\subset\mathbb{R}^3$ denote $I_B(\mathbf{x},\mathbf{y})=\int_B F(\mathbf{x},\mathbf{y},\mathbf{z})\,d\mathbf{z}$. Then

$$|I(\mathbf{x},\mathbf{y})-I(\mathbf{x}_0,\mathbf{y}_0)|\leqslant|I_{B_1(\eta)}(\mathbf{x},\mathbf{y})|+|I_{B_1(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|+|I_{B_2(\eta)}(\mathbf{x},\mathbf{y})-I_{B_2(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|\,.$$

If $\mathbf{x},\mathbf{y},\mathbf{z}\in B_1(\eta)$, then by (G2)

$$|F(\mathbf{x},\mathbf{y},\mathbf{z})|\leqslant f(\mathbf{z})\,|\mathbf{x}-\mathbf{y}|^{-1}|\mathbf{z}-\mathbf{y}|^{-1},$$

where $f\in L^p$, therefore relation (5) and the Cauchy–Schwartz inequality lead to the estimate $|I_{B_1(\eta)}(\mathbf{x},\mathbf{y})|+|I_{B_1(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|\leqslant\text{const}\,\eta$. On the other hand, if $\mathbf{x},\mathbf{y}\in B_1(\eta/2)$, $\mathbf{z}\in B_2(\eta)$, then we have from (G3): $|F(\mathbf{x},\mathbf{y},\mathbf{z})|\leqslant g(\mathbf{z})\exp(-\delta|\mathbf{z}|)$, where $\delta>0$ and $g\in L^p$. Thus by (G1) and the Lebesgue majorization theorem, $I_{B_2(\eta)}(\mathbf{x},\mathbf{y})$ is a continuous function on $B_1(\eta/2)\times B_1(\eta/2)$, and the proof of continuity of G^0_{reg} is completed.

Let $\mathbf{q}\in\mathbb{R}^3$, then the restriction of H^0 to the domain $\{f\in\mathcal{D}(H^0):f(\mathbf{q})=0\}$ is a closed symmetric operator S with the deficiency indices (1,1). By definition, the *point perturbation of* H^0, *supported on* $\mathbf{q}$ is a self-adjoint extension of S different from H^0. All the point perturbations of H^0 supported on a given $\mathbf{q}\in\mathbb{R}^3$ form a one-parameter family $H_\alpha(\mathbf{q})$, $\alpha\in\mathbb{R}$, of self-adjoin operators such that the Green function G_α of $H_\alpha(\mathbf{q})$ is given by the formula

$$G_\alpha(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\mathbf{y};\zeta)-[Q(\zeta;\mathbf{q})-\alpha]^{-1}G^0(\mathbf{x},\mathbf{q};\zeta)G^0(\mathbf{q},\mathbf{y};\zeta)\,, \tag{6}$$

which is a consequence of the Krein resolvent formula. Here $Q(\zeta;\mathbf{q})=G^0_{\text{reg}}(\mathbf{q},\mathbf{q};\zeta)$ is the so-called Krein $\mathcal{Q}$-function. The operator H^0 corresponds formally to $\alpha=\infty$; moreover, H^0 is the Friedrichs extension of S.

The extension parameter α has an important physical meaning, namely, H_α can be treated as the Hamiltonian H^0 perturbed by a zero-range potential, in this case α is the strength of this potential.[8,35,36] In place of the strength α, it is more convenient to use for applications so-called ''scattering length'' ℓ_s, $\ell_s=1/(4\pi\alpha)$ (see in Refs. 8, 35, and 36 again). More precisely,

$$\ell_s=\frac{\mu}{2\pi\hbar^2\alpha},$$

and we see that ℓ_s has actually the dimension of the length.

Note that according to the general results of the Krein self-adjoint extension theory, the function $\zeta \mapsto Q(\zeta;\mathbf{q})$ is analytic in the domain $\mathbb{C}\backslash\mathrm{spec}(H^0)$ for each $\mathbf{q}\in\mathbb{R}^3$ and $\partial Q(E;\mathbf{q})/\partial E>0$ if $E\in\mathbb{R}\backslash\mathrm{spec}(H^0)$.[37] Remark that $Q(\zeta;\mathbf{q})$ can be continuously extended to some points of $\mathrm{spec}(H^0)$. Further we assume that $Q(\zeta;\mathbf{q})$ is continuously extended to all regular points.

It is easy to prove that for every $\mathbf{q}\in\mathbb{R}^3$ the mapping $\zeta\mapsto G^0(\cdot,\mathbf{q};\zeta)$ is an analytic function from the domain $\mathbb{C}\backslash\mathrm{spec}\,(H^0)$ to the Hilbert space $L^2(\mathbb{R}^3)$. Denote $G^0(\cdot,\mathbf{q};\zeta)$ by $g_{\mathbf{q}}(\zeta)$, then we can rewrite (6) in an operator form

$$R_\alpha(\zeta)=R^0(\zeta)-[Q(\zeta;\mathbf{q})-\alpha]^{-1}|g_{\mathbf{q}}(\zeta)\rangle\langle g_{\mathbf{q}}(\zeta)|\,, \tag{7}$$

where $R_\alpha(\zeta)=(H_\alpha-\zeta)^{-1}$ and $R^0(\zeta)=(H^0-\zeta)^{-1}$.

Note, that $g_{\mathbf{q}}(\zeta)$ is a nonzero function for every $\mathbf{q}\in\mathbb{R}^3$ and $\zeta\in\mathbb{C}\backslash\mathrm{spec}\,(H^0)$. Indeed, otherwise we have $\varphi(\mathbf{q})=0$ for every $\varphi\in\mathcal{D}(H^0)$ that contradicts the inclusion $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)$.

In conclusion we mention a possibility to approximate the zero-range perturbation by potentials with decreasing support. For $V=0$ the corresponding procedure is described in Ref. 8 (Theorem 1.2.5). We sketch here the proof for H^0 with potential V having properties (P1), (P2).

Let $W\in L^2_{\mathrm{comp}}(\mathbb{R}^3)$, in particular, W is a Rollnik function (see in Ref. 32, Sec. X.2). Denote $v=|W|^{1/2}$, $u=v\,\mathrm{sign}(V)$, and let $\lambda(\varepsilon)$ be a real-analytic function in a neighborhood of zero such that $\lambda(0)=1$. For $\varepsilon>0$ consider the operator $H^\varepsilon\equiv H^\varepsilon(\mathbf{q})=H^0+\varepsilon^{-2}\lambda(\varepsilon)W(\varepsilon^{-1}(\mathbf{x}-\mathbf{q}))$. Then the resolvent $R^\varepsilon(\zeta)=(H^\varepsilon-\zeta)^{-1}$ $(\varepsilon>0)$ has the form

$$R^\varepsilon(\zeta)=R^0(\zeta)-\varepsilon\lambda(\varepsilon)A^\varepsilon[1+B^\varepsilon]^{-1}C^\varepsilon\,,$$

where A^ε, B^ε, C^ε are integral operators with the kernels $A^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\varepsilon\mathbf{y}+\mathbf{q};\zeta)v(\mathbf{y})$, $C^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=G^0(\varepsilon\mathbf{x}+\mathbf{q},\mathbf{y};\zeta)u(\mathbf{x})$, $B^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=\varepsilon\lambda(\varepsilon)G^0(\varepsilon\mathbf{x}+\mathbf{q},\varepsilon\mathbf{y}+\mathbf{q};\zeta)u(\mathbf{x})v(\mathbf{y})$. Define A^0 and C^0 putting $\varepsilon=0$ in the formulas above, and define B^0 by the integral kernel $B^0(\mathbf{x},\mathbf{y})=(4\pi|\mathbf{y}-\mathbf{x}|)^{-1}u(\mathbf{x})v(\mathbf{y})$. All the operators A^ε, B^ε and C^ε $(\varepsilon\geqslant 0)$ belong to the Hilbert–Schmidt class and $A^\varepsilon\to A^0$, $B^\varepsilon\to B^0$, $C^\varepsilon\to C^0$ with respect to the Hilbert–Schmidt norm as $\varepsilon\to+0$. Moreover, using (4) we can prove that with respect to this norm

$$B^\varepsilon=B^0+\varepsilon(\lambda'(0)B^0+Q(\zeta;\mathbf{q})|u\rangle\langle v|)+o(\varepsilon)\,.$$

Hence, the arguments using for the proof of Theorem 1.2.5 from Ref. 8 give the following result.

Theorem A:

(1) *Let* $\langle v|\varphi\rangle=0$ *for all* L^2*-solutions* φ *of the equation* $B^0\varphi=-\varphi$ *(in particular, let* -1 *be not an eigenvalue of* B_0*). Then* $H^\varepsilon(\mathbf{q})\to H^0$ *in the norm-resolvent sense as* $\varepsilon\to+0$;

(2) *let* -1 *be a simple eigenvalue of* B^0 *and* φ *be a corresponding eigenfunction normalized by the condition* $\langle\tilde\varphi|\varphi\rangle=-1$, *where* $\tilde\varphi=\varphi\,\mathrm{sign(V)}$. *If* $\langle v|\varphi\rangle\neq 0$, *then* $\lim_{\varepsilon\to+0}H^\varepsilon(\mathbf{q})=H_\alpha(\mathbf{q})$ *in the norm-resolvent sense, where* $\alpha=-\lambda'(0)|\langle v|\varphi\rangle|^{-2}$;

(3) *let* -1 *be a multiple eigenvalue of* B^0 *with eigenfunctions* $\varphi_1,\ldots,\varphi_n$ *normalized by the conditions* $\langle\tilde\varphi_j|\varphi_k\rangle=-\delta_{jk}$ $(\tilde\varphi_j=\varphi_j\,\mathrm{sign(V)})$. *If* $\langle v|\varphi_j\rangle\neq 0$ *for some* j *and* $\lambda'(0)\neq 0$, *then* $\lim_{\varepsilon\to+0}H^\varepsilon(\mathbf{q})=H_\alpha(\mathbf{q})$ *in the norm-resolvent sense, where*

$$\alpha=-\lambda'(0)\left[\sum_{j=1}^n|\langle v|\varphi_j\rangle|^2\right]^{-1}.$$

■

III. POINT PERTURBATION IN THE CASE OF UNBOUNDED POTENTIAL *V*

Starting with this section we suppose additionally that

(P3) $\lim_{|\mathbf{r}|\to\infty}V(\mathbf{r})=+\infty$.

In this case $R^0(\zeta)$ is a compact operator for all $\zeta\in\mathbb{C}\backslash\mathrm{spec}(H^0)$ (the Strichartz theorem; see, e.g., in Ref. 38, Theorem XIII.69). Therefore, $\mathrm{spec}(H^0)$ consists of an unbounded sequence $\lambda_0<\lambda_1<\cdots<\lambda_n<\cdots$ of eigenvalues with finite multiplicity k_n. Consequently, $Q(\zeta;\mathbf{q})$ is a meromorphic function of ζ. We are going to find the poles of this function.

Denote by L_n the eigenspace associated with λ_n, and choose in L_n an orthonormal basis $F_{n,k}(\mathbf{r})$, $k=1,\ldots,k_n$. For every $\mathbf{q}\in\mathbb{R}^3$ we denote

$$\sigma(\mathbf{q})=\{\lambda_n\in\mathrm{spec}(H^0):\exists f\in L_n \quad \text{s.t.} \quad f(\mathbf{q})\neq 0\}$$

Lemma 1: The set of all poles of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ coincides with $\sigma(\mathbf{q})$.

Proof: Since $(\partial G^0/\partial\zeta)(\mathbf{x},\mathbf{y};\zeta)$ is the integral kernel for the operator $(H^0-\zeta)^{-2}$, we have according to the Mercer theorem

$$\frac{\partial}{\partial\zeta}G^0(\mathbf{x},\mathbf{y};\zeta)=\sum_{n=0}^{\infty}\sum_{k=1}^{k_n}(\lambda_n-\zeta)^{-2}F_{n,k}(\mathbf{x})\overline{F_{n,k}(\mathbf{y})},$$

where the series converges locally uniformly on $\mathbb{R}^3\times\mathbb{R}^3\times(\mathbb{C}\backslash\mathrm{spec}(H^0))$. Therefore,

$$\frac{\partial}{\partial\zeta}Q(\zeta;\mathbf{q})=\sum_{n=0}^{\infty}\sum_{k=1}^{k_n}(\lambda_n-\zeta)^{-2}|F_{n,k}(\mathbf{q})|^2, \tag{8}$$

and the series converges locally uniformly on $(\mathbb{C}\backslash\mathrm{spec}(H^0))\times\mathbb{R}^3$. The lemma follows from (8) immediately. ■

Lemma 2: For each $\mathbf{q}\in\mathbb{R}^3$ the set $\sigma(\mathbf{q})$ is infinite. If V is bounded from below, then $\lambda_0\in\sigma(\mathbf{q})$.

Proof: Consider the space of continuous functions $C(\mathbb{R}^3)$ with the topology of compact convergence. Due to the closed graph theorem and the relation $\mathcal{D}(H^0)\subset C(\mathbb{R}^3)$, the operator $R^0(-1): L^2(\mathbb{R}^3)\to C(\mathbb{R}^3)$ is continuous. Therefore, for every $f\in\mathcal{D}(H^0)$ the Fourier expansion for f with respect to the basis $(F_{n,k})_{n,k}$ converges locally uniformly. Assume that the set $\sigma(\mathbf{q})$ is finite; let $N=\max\{n:\lambda_n\in\sigma(\mathbf{q})\}$ and P be the orthogonal projection of $L^2(\mathbb{R}^3)$ on the subspace $M=L_0+\ldots+L_N$. Then for every $\varphi\in\mathcal{D}(H^0)$ the conditions $\varphi(\mathbf{q})=0$ and $(P\varphi)(\mathbf{q})=0$ are equivalent. Since M is finite dimensional, there is $h\in M$ such that for every $\varphi\in M$ the conditions $\varphi(\mathbf{q})=0$ and $\langle h|\varphi\rangle=0$ are also equivalent. Using the inclusion $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)$ we see that there is a function $h\in L^2(\mathbb{R}^3)$ such that for every $\varphi\in C_0^\infty(\mathbb{R}^3)$ the conditions $\varphi(\mathbf{q})=0$ and $\langle h|\varphi\rangle=0$ are equivalent. Obviously, this is impossible, hence $\sigma(\mathbf{q})$ is infinite. If V is bounded from below, then by Theorem XIII.48 from Ref. 38 the eigenfunctions of H^0 corresponding to the ground state λ_0 have no zeros therefore $\lambda_0\in\sigma(\mathbf{q})$. ■

Another property of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ we need further follows.

Lemma 3: The function $Q(\zeta;\mathbf{q})$ tends to $-\infty$ as $\zeta\to-\infty$, $\zeta\in\mathbb{R}$.

Proof: Since H^0 is the Friedrichs extension of S, the statement follows from Proposition 4 of Ref. 39. ■

IV. SPECTRAL PROPERTIES OF H_α AT FIXED POSITION OF THE POINT PERTURBATION

Here we describe the spectrum of $H_\alpha(\mathbf{q})$ for a fixed $\mathbf{q}\in\mathbb{R}^3$. Further, if it does not lead to a misunderstanding, we omit $\mathbf{q}$ from the notations.

Since H_α is a rank one perturbation of H^0, the spectrum of H_α is discrete. Moreover, an eigenvalue λ_n of H^0 of the multiplicity k_n is an eigenvalue of H_α of the multiplicity k_n-1, k_n or k_n+1 [if $k_n=1$, the first case means, of course, that λ_n does not belong to $\mathrm{spec}(H_\alpha)$]. For $\lambda\notin\mathrm{spec}(H^0)$ we see from (7) that λ is an eigenvalue of H_α if and only if $\zeta=\lambda$ is a solution to the equation

$$Q(\zeta;\mathbf{q})-\alpha=0. \tag{9}$$

Denote by $(\varepsilon_n)_{n\in\mathbb{N}}=(\varepsilon_n(\mathbf{q}))_{n\in\mathbb{N}}$ the strictly increasing sequence of all the poles of $Q(\zeta;\mathbf{q})$. Since $(\partial Q/\partial E)(E;\mathbf{q})>0$ for $E\in\mathbb{R}\setminus\mathrm{spec}(H^0)$, Eq. (9) has exactly one solution on each interval $(-\infty,\varepsilon_0),(\varepsilon_0,\varepsilon_1),\ldots$. Denote such solutions, which do not belong to $\mathrm{spec}(H^0)$, by $\mathcal{E}_0,\mathcal{E}_1,\ldots$, where $\mathcal{E}_0<\mathcal{E}_1<\cdots$. The following theorem completely describes the eigenvalues and the eigenfunctions of $H_\alpha(\mathbf{q})$.

Theorem 1: *Let $\mathbf{q}\in\mathbb{R}^3$ be fixed. The spectrum of $H_\alpha=H_\alpha(\mathbf{q})$ is discrete and consists of four nonintersecting parts $\sigma_1,\sigma_2,\sigma_3,\sigma_4$ described as follows.*

(1) σ_1 is the set of all solutions $\mathcal{E}_n$ to the Eq. (9), which do not belong to $\mathrm{spec}(H^0)$. The multiplicity of $\mathcal{E}_n$ in the spectrum of H^0 is equal to 1.
(2) σ_2 is the set of all $\lambda_n\in\sigma(\mathbf{q})$ that are multiple eigenvalues of H^0. The multiplicity of the eigenvalue $\lambda_n\in\sigma_2$ in the spectrum of H_α is equal to k_n-1.
(3) σ_3 consists of all λ_n, $\lambda_n\in\mathrm{spec}\,(H^0)\setminus\sigma(\mathbf{q})$, that are not solutions of (9). The multiplicity of the eigenvalue λ_n in $\mathrm{spec}(H_\alpha)$ is equal to k_n.
(4) σ_4 consists of all λ_n, $\lambda_n\in\mathrm{spec}\,(H^0)\setminus\sigma(\mathbf{q})$, such that λ_n is a solution of (9). The multiplicity of the eigenvalue λ_n in $\mathrm{spec}(H_\alpha)$ is equal to k_n+1.

The corresponding eigensubspaces are described as follows.

(1) The subspace spanned by the normalized eigenfunction
$$\Phi_n=\left[\frac{\partial Q}{\partial\zeta}(\mathcal{E}_n;\mathbf{q})\right]^{-1/2}g_{\mathbf{q}}(\mathcal{E}_n)\,.$$
(2) The orthogonal complement in L_n of the function
$$\Psi_n(\mathbf{x})=\sum_{k=1}^{k_n}\overline{F_{n,k}(\mathbf{q})}F_{n,k}(\mathbf{x})\,,$$
or, equivalently, the subspace of L_n of the form $\{f\in L_n: f(\mathbf{q})=0\}$.
(3) The subspace L_n.
(4) The direct sum of L_n and the space spanned by the function $g_{\mathbf{q}}(\lambda_n)$, which is orthogonal to L_n.

Proof: The proof is based on direct calculations with the help of following statements:
(A) *The orthoprojector $P(E_0)$ on the eigenspace of a self-adjoint operator T corresponding to an isolated eigenvalue E_0 has the form*
$$P(E_0)=-\mathrm{Res}[(T-\zeta)^{-1};\zeta=E_0].$$
(B) *Suppose P_1,P_2 and P_1+cP_2, where $c\in\mathbb{C}$, are orthoprojectors in a Hilbert space and $P_2\neq 0$, then c equals 0, 1 or -1.*

The first statement is well known; we omit the easy proof of the second one. Denote by $A(\zeta)$,
$$A(\zeta)=[Q(\zeta;\mathbf{q})-\alpha]^{-1}|g_{\mathbf{q}}(\zeta)\rangle\langle g_{\mathbf{q}}(\zeta)|,$$
the second term in the representation (7) of the resolvent. Further, denote for $E_0\in\mathbb{R}$
$$P_\alpha(E_0)=-\mathrm{Res}[R_\alpha(\zeta);\zeta=E_0]\,,$$
$$P^0(E_0)=-\mathrm{Res}[R^0(\zeta);\zeta=E_0]\,,$$
$$T(E_0)=\mathrm{Res}[A(\zeta);\zeta=E_0]\,;$$
therefore, according to (7)
$$P_\alpha(E_0)=P^0(E_0)+T(E_0)\,.$$

Start with the proof of the first assertion of Theorem. It is obvious that $\sigma_1 \subset \mathrm{spec}(H_\alpha)$. Let $\mathcal{E}_n \in \sigma_1$, then in a vicinity of $\mathcal{E}_n$ we have the following expansion:

$$Q(\zeta;\mathbf{q}) - \alpha = \frac{\partial}{\partial\zeta} Q(\mathcal{E}_n;\mathbf{q})(\zeta - \mathcal{E}_n) + O(\zeta - \mathcal{E}_n)^2. \tag{10}$$

Therefore,

$$T(\mathcal{E}_n) = \left[\frac{\partial}{\partial\zeta} Q(\mathcal{E}_n;\mathbf{q})\right]^{-1} |g_{\mathbf{q}}(\mathcal{E}_n)\rangle\langle g_{\mathbf{q}}(\mathcal{E}_n)| \,. \tag{11}$$

Since obviously $P^0(\mathcal{E}_n) = 0$, we have $P_\alpha(\mathcal{E}_n) = T(\mathcal{E}_n)$ and the normalized eigenfunction corresponding to $\mathcal{E}_n$ is

$$\Phi_n = \left[\frac{\partial Q}{\partial\zeta}(\mathcal{E}_n;\mathbf{q})\right]^{-1/2} g_{\mathbf{q}}(\mathcal{E}_n) \,. \tag{12}$$

Now consider an eigenvalue λ_n of H^0. In this case $P_\alpha(\lambda_n) = P^0(\lambda_n) + T(\lambda_n)$. According to (8), in a neighborhood W of λ_n we have the following representation

$$g_{\mathbf{q}}(\zeta) = \Psi_n(\cdot;\mathbf{q})(\lambda_n - \zeta)^{-1} + f(\zeta) \,,$$

where f is analytic function in W with values in $L^2(\mathbb{R}^3)$ and

$$\Psi_n(\mathbf{x};\mathbf{q}) = \sum_{k=1}^{k_n} \overline{F_{n,k}(\mathbf{q})} F_{n,k}(\mathbf{x}) \,.$$

Consider the following three cases: (a) $\lambda_n \in \sigma(\mathbf{q})$; (b) $\lambda_n \notin \sigma(\mathbf{q})$ and $Q(\lambda_n;\mathbf{q}) - \alpha \neq 0$; (c) $\lambda_n \notin \sigma(\mathbf{q})$ and $Q(\lambda_n;\mathbf{q}) - \alpha = 0$.

Let us start with the case (a). Since λ_n is a pole of $Q(\cdot;\mathbf{q})$, we have $\Psi_n(\cdot;\mathbf{q}) \neq 0$ and therefore $T = cP$, where P is the orthoprojector on the one-dimensional space spanned by $\Psi_n(\cdot;\mathbf{q})$. Since $\Psi_n(\cdot;\mathbf{q}) \in L_n$, in virtue of statement (B) $c = -1$, and the assertion (2) of Theorem is proven.

In the case (b) according to Lemma 1, $F_{n,k}(\mathbf{q}) = 0$ for all $k = 1,\ldots,k_n$; hence $\Psi_n(\cdot,\mathbf{q}) = 0$ and $T(\lambda_n) = 0$. This implies assertion (3) of Theorem.

Finally, in the case (c) we can use (10)–(12) with $\zeta = \lambda_n$ instead of $\zeta = \mathcal{E}_n$, and obtain

$$T(\lambda_n) = |\Phi_n\rangle\langle\Phi_n| \,,$$

according to (B), this get the statement (4) of Theorem. ■

For $n \in \mathbb{N}$ denote by A_n the set of all $\alpha \in \mathbb{R}$ such that the solution $\mathcal{E}_n \equiv \mathcal{E}_n(\alpha)$ of Equation (9) does not belong to the spectrum of H^0. Lemma 2 shows that $\mathbb{R} \backslash A_n$ is finite, moreover, if V bounded from below, then $A_0 = \mathbb{R}$.

For all $\mathbf{q} \in \mathbb{R}^3$ we will denote $\varepsilon_{-1}(\mathbf{q}) = \lambda_{-1} = -\infty$. Using Lemmas 1 and 3 we get immediately the following proposition.

Proposition 1: For each $n \in \mathbb{N}$ the function $\alpha \mapsto \mathcal{E}_n(\alpha)$ strictly increases on A_n. Moreover,

$$\lim_{\alpha\to+\infty} \mathcal{E}_n(\alpha) = \varepsilon_n \,, \qquad \lim_{\alpha\to-\infty} \mathcal{E}_n(\alpha) = \varepsilon_{n-1} \,.$$

■

Remark: For $n = 0$ we have an interesting phenomenon of falling the considered particle on the point $\mathbf{q}$ (the falling on the attractive center; cf. Ref. 21 for the case of a one-dimensional oscillator). Indeed, using estimate (b′) from Theorem B.7.1 of Ref. 31, we obtain without any difficulty $|\Phi_0(\mathbf{x})|^2 \to \delta(\mathbf{x} - \mathbf{q})$ in an appropriate space of distributions as $\alpha \to -\infty$ (and therefore

$\mathcal{E}_0 \to -\infty$). According to the standard interpretation of quantum mechanics, this relation means that the probability to find the particle in a domain not containing the point $\mathbf{q}$ tends to zero as $\mathcal{E}_0$ tends to $-\infty$.

V. DEPENDENCE OF THE SPECTRUM OF $H_\alpha(\mathbf{q})$ ON q

Here we are going to analyze the dependence of the eigenvalues of H_α on $\mathbf{q}$. It is clear that $\mathcal{E}_n(\mathbf{q})$ are continuous branches of the multi-valued function defined by Eq. (9). This branches can intersect at values λ_n where a monodromy arises. To get a univalent enumeration of these branches, we modify the parametrization of the eigenvalues of H_α given by Theorem 1 (the enumeration of the numbers $\mathcal{E}_n(\mathbf{q})$ depends on the enumeration of poles $\varepsilon_n \in \mathrm{spec}(H^0)$, which in its turn depends obviously on $\mathbf{q}$). For $n=-1,0,\ldots$ consider the sets X_n defined as follows: $X_{-1}=\mathbb{R}^3$, and

$$X_n=\{\mathbf{q}\in\mathbb{R}^3:\exists f\in L_n \ \text{ s.t. } \ f(\mathbf{q})\neq 0\}=\{\mathbf{q}\in\mathbb{R}^3:\lambda_n\in\sigma(\mathbf{q})\},$$

for $n\geqslant 0$. For all $n\in\mathbb{N}$ the set $\mathbb{R}^3\backslash X_n$ is nowhere dense in $\mathbb{R}^3$ (see in Ref. 38, Theorem XIII.63). According to Lemma 1, for $n\geqslant 0$, the set X_n coincides with the set of all $\mathbf{q}\in\mathbb{R}^3$ such that λ_n is a pole of the function $Q(\cdot;\mathbf{q})$. Since we do not suppose the potential V is smooth, the function $Q(\zeta;\mathbf{q})$ on the set $(\lambda_{n-1},\lambda_n)\times(X_{n-1}\cap X_n)$, $n\geqslant 0$, is not, generally speaking, smooth. Nevertheless, it is monotone and real analytic with respect to the first argument ζ and continuous with respect to the second argument $\mathbf{q}$. In this case the following simple variant of Implicit Function Theorem is applicable (see in Ref. 40 for the proof):

Let J be an open nonempty interval of the real line $\mathbb{R}$, X be a topological space, and $F\colon J\times X\to\mathbb{R}$ be a separately continuous function such that each partial function $t\mapsto F(t,x)$, $x\in X$, is strictly monotone. Suppose that $F(t_0,x_0)=0$ for some $(t_0,x_0)\in J\times X$. Then there are an open neighborhood U of the point x_0 in X and a continuous function $f\colon U\to J$ such that (1) $F(f(x),x)=0$ for all $x\in U$; (2) if U' is another neighborhood of x_0, and $g\colon U'\to J$ is a function with the property: $F(g(x),x)=0$ for all $x\in U'$, then $U'\subset U$, and $f_{|U'}=g$.

According to this version of Implicit Function Theorem, for any $\mathbf{q}\in X_{n-1}\cap X_n$ there exists a unique solution $E_n(\mathbf{q})$ to Eq. (9) that belongs to $(\lambda_{n-1},\lambda_n)$ and $\mathbf{q}\mapsto E_n(\mathbf{q})$ is a continuous function in $X_{n-1}\cap X_n$.

Proposition 2: Every function $E_n(\mathbf{q})$, $n=0,1,\ldots$, has a continuous extension to the whole space $\mathbb{R}^3$.

Proof: Fix $n=0,1,\ldots$, and let a point $\mathbf{q}$, $\mathbf{q}\in\mathbb{R}^3\backslash(X_{n-1}\cap X_n)$, be given. Choose a sequence $(\mathbf{q}_k)_{k\in\mathbb{N}}$ from $X_{n-1}\cap X_n$ which tends to $\mathbf{q}$. First we note that the sequence $(E_n(\mathbf{q}_k))_{k\in\mathbb{N}}$ is bounded in $\mathbb{R}$. It is trivial for $n>0$. If $n=0$, the sequence is bounded from above. We prove that it is bounded from below as well. Otherwise $E_0(\mathbf{q}_{k_l})\to-\infty$ for some subsequence $(\mathbf{q}_{k_l})$. Since $Q(E;\mathbf{q})\to-\infty$ as $E\to-\infty$, there exists $A<\lambda_0$ such that $Q(A;\mathbf{q})<\alpha$. Then there exists $N\in\mathbb{N}$ such that $Q(A;\mathbf{q}_{k_l})<\alpha$ and $E_0(\mathbf{q}_{k_l})<A$ if $l\geqslant N$. Therefore, for $k\geqslant N$ we have

$$Q(E_0(\mathbf{q}_{k_l});\mathbf{q}_{k_l})-\alpha< Q(A;\mathbf{q}_{k_l})-\alpha<0,$$

and we get a contradiction with the definition of $E_0(\mathbf{q}_{k_l})$.

By Bolzano–Weierstrass we can extract a subsequence $(\mathbf{q}_{k_l})$ from the sequence $(\mathbf{q}_k)$ such that the subsequence $(E_n(\mathbf{q}_{k_l}))$ has a limit, which we denote by E'. To prove that the sequence $(E_n(\mathbf{q}_k))$ tends to E' and E' is independent of the choice of a sequence $(\mathbf{q}_k)$ tending to $\mathbf{q}$ we need the following lemma concerning properties of E'.

Lemma 5: The limit E' has the properties:

(1) E' is not a pole of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$;
(2) if $\lambda_{n-1}<E'<\lambda_n$, then E' is a unique solution of Eq. (9) in the interval $(\lambda_{n-1},\lambda_n)$;
(3) if $E'=\lambda_{n-1}$, then $\lim_{E\to E'}[Q(E;\mathbf{q})-\alpha]\geqslant 0$;
(4) if $E'=\lambda_n$, then $\lim_{E\to E'}[Q(E;\mathbf{q})-\alpha]\leqslant 0$.

Proof of the lemma:

(1) First consider the case $n>0$. The function $\tilde{Q}_n(\zeta;\mathbf{q})=[Q(\zeta;\mathbf{q})-\alpha](\zeta-\lambda_{n-1})(\zeta-\lambda_n)$ is continuous on the interval $(\lambda_{n-2},\lambda_{n+1})\times\mathbb{R}^3$. Since $\tilde{Q}_n(E_n(\mathbf{q}_{k_l});\mathbf{q}_{k_l})=0$, passing to the limit $l\to\infty$ we get $\tilde{Q}_n(E';\mathbf{q})=0$. Suppose $\zeta=E'$ is a pole of $Q(\zeta;\mathbf{q})$, then $\tilde{Q}_n(E';\mathbf{q})=\mathrm{Res}[Q(\zeta;\mathbf{q});\zeta=E']\neq 0$, and we get a contradiction. For $n=0$, we consider $\tilde{Q}_0(\zeta;\mathbf{q})=[Q(\zeta;\mathbf{q})-\alpha](\zeta-\lambda_0)$, and get the same result.

(2) It is sufficient to pass to the limit $l\to\infty$ in the identity $Q(E_n(\mathbf{q}_{k_l});\mathbf{q}_{k_l})=0$.

(3) In virtue of statement (1) of the lemma, the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ is continuous in a neighborhood of E', and therefore there exists a limit $\lim_{\zeta\to\lambda_{n-1}}[Q(\zeta;\mathbf{q})-\alpha]=L$. Assume that $L<0$, then $Q(E,\mathbf{q})-\alpha<0$ for some $E\in(\lambda_{n-1},\lambda_n)$. Choose some m such that $E_n(\mathbf{q}_{k_m})<E$. Since $Q(\zeta;\mathbf{q})$ increases on the interval $(\lambda_{n-1},\lambda_n)$ as the function of ζ, we obtain a contradiction:

$$0=Q(E_n(\mathbf{q}_{k_m});\mathbf{q}_{k_m})-\alpha<Q(E;\mathbf{q}_{k_m})-\alpha<0\ .$$

Statement (4) can be proven similarly to (3). ■

Let us return to the proof of the proposition. We prove that if a sequence $(\mathbf{p}_k)_{k\in\mathbb{N}}$ from $X_{k-1}\cap X_k$ converges to the point $\mathbf{q}$, then $E_n(\mathbf{p}_k)\to E'$.

Suppose $E_n(\mathbf{p}_k)$ does not converge to E', then there exists a subsequence $(\mathbf{p}_{k_l})$ such that $E_n(\mathbf{p}_{k_l})\to E^*$, $E^*\neq E'$. Assume $E^*<E'$. Taking into account item (2) of Lemma 5 we get $E^*=\lambda_{n-1}$ or $E'=\lambda_n$. In both the cases we have

$$\lim_{\zeta\to E^*}[Q(\zeta;\mathbf{q})-\alpha]\geqslant 0 \quad \text{and} \quad \lim_{\zeta\to E'}[Q(\zeta;\mathbf{q})-\alpha]\leqslant 0.$$

Take some real numbers E_1 and E_2 such that $E^*<E_1<E_2<E'$. Then by the strict monotonicity of $\zeta\mapsto Q(\zeta;\mathbf{q})$ we have

$$0\leqslant Q(E_1;\mathbf{q})-\alpha<Q(E_2,\mathbf{q})-\alpha\leqslant 0\ .$$

This is a contradiction. ■

The following theorem is the main result of this section.

Theorem 2: *For each fixed $\alpha\in\mathbb{R}$ there is a sequence $(E_n(\mathbf{q}))_{n\in\mathbb{N}}$ of continuous functions of $\mathbf{q}\in\mathbb{R}^3$ with the following properties:*

(1) $\lambda_{n-1}\leqslant E_n(\mathbf{q})\leqslant\lambda_n$ for all $n\in\mathbb{N}$.

(2) For each $\mathbf{q}\in\mathbb{R}^3$ the set consisting of all $E_n(\mathbf{q})$ and all the numbers λ_n with multiplicities $k_n>1$ form the complete collection of the eigenvalues of the operator $H_\alpha(\mathbf{q})$.

(3) If $\lambda_{n-1}<E_n(\mathbf{q})<\lambda_n$, then $E_n(\mathbf{q})$ is a unique solution of the Eq. (9) on the interval $(\lambda_{n-1},\lambda_n)$.

(4) If $\zeta=\lambda_n$ is a pole of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$, then $E_{n-1}(\mathbf{q})<\lambda_n<E_n(\mathbf{q})$.

(5) If $\zeta=\lambda_n$ is not a pole of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$, then we have the following assertions:

(a) if $Q(\lambda_n;\mathbf{q})-\alpha<0$, then $E_n(\mathbf{q})=\lambda_n<E_{n+1}(\mathbf{q})$;

(b) if $Q(\lambda_n;\mathbf{q})-\alpha>0$, then $E_n(\mathbf{q})<\lambda_n=E_{n+1}(\mathbf{q})$;

(c) if $Q(\lambda_n;\mathbf{q})-\alpha=0$, then $E_n(\mathbf{q})=\lambda_n=E_{n+1}(\mathbf{q})$.

Proof: Consider the functions $E_n(\mathbf{q})$ given by Proposition 2. Then (1) is obvious by definition of $E_n(\mathbf{q})$. Assertion (2) follows from Theorem 1. Assertions (3) and (4) were proven in Lemma 5. It remains to prove (5).

Let λ_n be not a pole of $\zeta\mapsto Q(\zeta;\mathbf{q})$. Suppose $Q(\lambda_n;\mathbf{q})-\alpha<0$. For any positive integer m we choose a number E'_m such that $\lambda_n-1/m<E'_m<\lambda_n$; then $Q(E'_m;\mathbf{q})-\alpha<0$. Further, we choose points $\mathbf{q}_m\in\mathbb{R}^3$ such that λ_{n-1} and λ_n are not poles of the function $\zeta\mapsto Q(\zeta;\mathbf{q}_m)$ (that is $\mathbf{q}_m\in X_{m-1}\cap X_m$), and such that $|\mathbf{q}-\mathbf{q}_m|<1/m$ and $Q(E'_m;\mathbf{q}_m)-\alpha<0$. Then $\zeta=E_n(\mathbf{q}_m)$ is a solution of the equation $Q(\zeta;\mathbf{q}_m)-\alpha=0$ lying in the interval $(\lambda_{n-1},\lambda_n)$. Since $Q(\zeta;\mathbf{q}_m)$ is a strictly monotone function of ζ on this interval, the inequalities $E'_m<E_n(\mathbf{q}_m)<\lambda_n$ take place for all m. Thus $E_n(\mathbf{q}_m)\to\lambda_n$ and $\mathbf{q}_m\to\mathbf{q}$ as $m\to\infty$; therefore, $\lambda_n=E_n(\mathbf{q})$ by the definition of the function $E_n(\mathbf{q})$. According to Lemma 5, $Q(\lambda_n;\mathbf{q})-\alpha\geqslant 0$, if $\lambda_n=E_{n+1}(\mathbf{q})$; therefore $\lambda_n<E_{n+1}(\mathbf{q})$. Hence, item (5a) is proved. The proofs of items (5b) and (5c) are similar. ■

Theorem 2 gives a useful description of the spectrum of H_α. Namely, denote by M the set $\{m\in\mathbb{N}: k_m>1\}$ and together with the functions $E_n(\mathbf{q})$ introduce a sequence of constant functions $\Lambda_m^{(k)}(\mathbf{q})=\lambda_m$, where $m\in M$, $k=1,\ldots,k_m-1$. Then $E_n(\mathbf{q})\leqslant\Lambda_n^{(k)}(\mathbf{q})\leqslant E_{n+1}(\mathbf{q})$ for all $n\in M$, $k=1,\ldots,k_n-1$, and for any fixed $\mathbf{q}\in\mathbb{R}^3$ the union of the sequences $(E_n(\mathbf{q}))_{n\in\mathbb{N}}$ and $(\Lambda_m^{(k)}(\mathbf{q}))_{m\in M,k=1,\ldots,k_m-1}$ forms the complete set of the eigenvalues of $H_\alpha(\mathbf{q})$ multiplicity counting. If $\mathbf{q}\in\cap_{n=0}^{\infty}X_n$, then every $E_n(\mathbf{q})$ is distinct from the numbers $\Lambda_m^{(k)}(\mathbf{q})$. Since $\mathbb{R}\backslash\cap_{n=0}^{\infty}X_n$ is the set of the first Baire category, for a generic $\mathbf{q}$ the point perturbation levels $E_n(\mathbf{q})$ are distinct from the levels of the unperturbed operator H^0.

VI. POINT PERTURBATIONS OF THE HARMONIC OSCILLATOR

Here we apply the results of the previous sections to the Hamiltonian (2) with the potential

$$V(\mathbf{r})=\frac{\mu\Omega_x^2}{2}x^2+\frac{\mu\Omega_y^2}{2}y^2+\frac{\mu\Omega_z^2}{2}z^2, \tag{13}$$

where Ω_j $(j=x,y,z)$ are the frequencies of the oscillator. The function V can be considered as a confinement potential of a quantum well in $\mathbb{R}^3$ with the characteristic sizes

$$L_j=\sqrt{\frac{\hbar}{2\mu\Omega_j}},\qquad j=x,y,z$$

(numbers $\sqrt{2}L_j$ are called also *length parameters* of the oscillator[41]). Therefore the operator with potential (13) can be used as the Hamiltonian of a (generally speaking, asymmetric) quantum dot.[1] It is convenient to pass to dimensionless coordinates $\mathbf{x}=\mathbf{r}/L$, where $L=\sqrt[3]{L_xL_yL_z}$. In the coordinates $\mathbf{x}=(x_1,x_2,x_3)$ the operator $\hat{H}^0$ takes the form $\hat{H}^0=\hbar\Omega H^0$, where

$$H^0=-\Delta+\tfrac{1}{4}(\omega_1^2x_1^2+\omega_2^2x_2^2+\omega_3^2x_3^2),$$

$$\Omega=\sqrt[3]{\Omega_x\Omega_y\Omega_z},\quad \omega_1=\frac{\Omega_x}{\Omega},\quad \omega_2=\frac{\Omega_y}{\Omega},\quad \omega_3=\frac{\Omega_z}{\Omega}$$

(hence, $\omega_1\omega_2\omega_3=1$).

Further we discuss the properties of H^0. The spectrum of this operator consists of the eigenvalues

$$\lambda_{n_1n_2n_3}=\omega_1(n_1+1/2)+\omega_2(n_2+1/2)+\omega_3(n_3+1/2),$$

where $n_1,n_2,n_3\in\mathbb{N}$. The corresponding normalized eigenfunctions are

$$\Phi_{n_1n_2n_3}(\mathbf{x})=\varphi_{n_1}(x_1)\varphi_{n_2}(x_2)\varphi_{n_3}(x_3),$$

where

$$\varphi_{n_j}(x_j)=\left(\frac{\omega_j}{2\pi}\right)^{1/4}(2^{n_j}n_j!)^{-1/2}\exp\left(-\frac{1}{4}\omega_jx_j^2\right)H_n\left(\sqrt{\frac{\omega_j}{2}}x_j\right)$$

is the oscillator function $[H_n(x)$ is the Hermite polynomial of degree $n]$.

If the frequencies $\omega_1, \omega_2, \omega_3$ are independent over the ring $\mathbb{Z}$ (this is the generic case), then the spectrum of H^0 is simple; therefore, the multiplicity of the eigenvalues of $H_\alpha(\mathbf{q})$ does not exceed 2 and the part σ_2 of the spectrum spec $(H_\alpha(\mathbf{q}))$ is always empty. On the other hand, since $H_n(0)=0$ if and only if n is odd, $\lambda_{n_1,n_2,n_3} \in \mathrm{spec}(H_\alpha(0))$ if and only if one of the numbers n_j $(j=1,2,3)$ is odd; hence, $\mathrm{spec}(H^0)\setminus\sigma(0)$ is always infinite. In addition, for all $n>0$ the set $\mathbb{R}^3\setminus X_n$ is infinite.

In general case, there are no explicit expressions for the Green functions of the harmonic oscillator in terms of commonly used elementary or special functions. Nevertheless, in a number of cases, the representation of the Green function $G^0(\mathbf{x},\mathbf{y};E)$ as the Laplace transform of the heat kernel $K(\mathbf{x},\mathbf{y};t)$ for H^0 is very useful to investigate some properties of the Krein $\mathcal{Q}$-function. The heat kernel for H^0 has the form (see, e.g., in Ref. 42):

$$K^0(\mathbf{x},\mathbf{y};t)=\prod_{j=1}^{3}\left(\frac{1}{4\pi \mathrm{sh}\omega_j t}\right)^{1/2}\exp\left(-\frac{\omega_j}{4\mathrm{sh}\omega_j t}((x_j^2+y_j^2)\mathrm{ch}\omega_j t-2x_j y_j)\right).$$

Using the heat kernel K^f for the free Hamiltonian $H^f=-\Delta$,

$$K^f(\mathbf{x},\mathbf{y};t)=(4\pi t)^{-3/2}\exp\left(-\frac{(\mathbf{x}-\mathbf{y})^2}{4t}\right),$$

and the $\mathcal{Q}$-function for H_f,

$$Q^f(\zeta)=-\frac{\sqrt{-\zeta}}{4\pi},$$

we get immediately from the formula

$$G(\mathbf{x},\mathbf{y};E)=\int_0^\infty e^{tE}K(\mathbf{x},\mathbf{y};t)\,dt,$$

that for $\mathrm{Re}\,\zeta<(\omega_1+\omega_2+\omega_3)/2$ the following representation of the $\mathcal{Q}$-function for H^0 takes place:

$$Q(\zeta;\mathbf{q})=-\frac{\sqrt{-\zeta}}{4\pi}+\frac{1}{(4\pi)^{3/2}}\int_0^\infty\left(\prod_{j=1}^{3}\left(\frac{1}{\mathrm{sh}\omega_j t}\right)^{1/2}\exp\left(-\frac{1}{2}q_j^2\omega_j \mathrm{th}\frac{\omega_j t}{2}\right)-\frac{1}{t^{3/2}}\right)e^{\zeta t}\,dt. \quad (14)$$

It is clear from (14) that $(\partial Q/\partial q_j)(E;\mathbf{q})<0$ for $q_j>0$, if $E<\lambda_0=(\omega_1+\omega_2+\omega_3)/2$. Since $\partial Q/\partial E>0$ for $E\in\mathbb{R}\setminus\mathrm{spec}\,(H^0)$, (9) implies that $\partial E_0/\partial q_j>0$. In particular, the depth of the lowest impurity level $\lambda_0-E_0(\mathbf{q})$ decreases if $|\mathbf{q}|$ increases in such a way that the inner product $\mathbf{a}\cdot\mathbf{q}$ remains positive for each vector $\mathbf{a}$ with positive coordinates. In the spherically symmetric case $\omega_1=\omega_2=\omega_3$, we have $\partial Q/\partial q<0$, where $q=|\mathbf{q}|>0$, and the depth decreases with increasing of q. This phenomenon was discovered numerically for a spherically symmetric quantum dot in Ref. 14 and called *positional disorder*. We see that the positional disorder is common to each parabolic quantum dot, not only to the spherically symmetric one. The similar result is valid in the two-dimensional case, i.e., for the case of impurities in a quantum well (see numerical results in Ref. 14). Our arguments are valid in the two-dimensional case also, thus we have a strict proof for the positional disorder in a two-dimensional quantum well.

The more detailed analysis is possible in the case of the *isotropic oscillator:* $\Omega_x=\Omega_y=\Omega_z$ $(=\Omega)$, i.e., in the case of a spherically symmetric quantum dot. In this case $\omega_1=\omega_2=\omega_3=1$ and the spectrum of H^0 consists of the eigenvalues

$$\lambda_n=n+\tfrac{3}{2},\quad n\in\mathbb{N},$$

where λ_n has the multiplicity $k_n=(n+1)(n+2)/2$. In this case there are natural units of length (namely, L) and of energy $(\hbar\Omega)$. Therefore, the following very important scaling properties takes place. Denote by $\hat{Q}(\zeta;\mathbf{q})$ the Krein $\mathcal{Q}$-function for the operator $\hat{H}^0$ keeping the notation $Q(\zeta;\mathbf{q})$ for the $\mathcal{Q}$-function of H^0. Then

$$\hat{Q}(\zeta;\mathbf{q})=\frac{1}{\hbar\Omega L^3}Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=4\pi\frac{\mu}{2\pi\hbar^2 L}Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right).$$

Denote $\mu/(2\pi\hbar^2 L)$ by α^0; obviously, α^0 is strength of the point potential corresponding to the scattering length L. Then Eq. (9) takes the form

$$4\pi Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=\frac{\alpha}{\alpha^0}, \tag{15}$$

or, equivalently,

$$4\pi Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=\frac{L}{\ell_s}.$$

Equation (15) shows that a change of the frequency Ω does not change the numerical values of energy levels in the spectrum of $\hat{H}^0$ if L is used as the unit of length, $\hbar\Omega$ as the unit of energy and α^0 as the unit of point potential strength.

In the case of isotropic oscillator, the set $\sigma(\mathbf{q})$ has a simple description:

Proposition 3: Let $\Omega_x=\Omega_y=\Omega_z$. *Then* $\sigma(\mathbf{q})=\{\lambda_{2n}: n\in\mathbb{N}\}$, *if* $\mathbf{q}=0$, *and* $\sigma(\mathbf{q})=\mathrm{spec}(H^0)$ *otherwise*.

Proof: Each λ_n is equal to $\lambda_{n_1n_2n_3}$, where $n_1+n_2+n_3=n$. If n is odd, then at least one of n_j is odd, and $\Psi_{n_1n_2n_3}(0)=0$. Therefore, $\lambda_n\notin\sigma(0)$. On the other hand, if n is even, then $\Psi_{n00}(0)\neq 0$, and therefore, $\lambda_n\in\sigma(0)$.

Let now $\mathbf{q}\neq 0$. First we remark that for all $n\in\mathbb{N}$ the following assertion is valid:

Lemma 6: If $H_n(x_0)=0$, *then* $H_{n+1}(x_0)\neq 0$.

Proof of the lemma: For all $n\in\mathbb{N}$ the following relation takes place:[43]

$$H'_{n+1}(x)=2(n+1)H_n(x).$$

If $H_n(x_0)=H_{n+1}(x_0)=0$, then $H'_n(x_0)=0$. Since $y=H_n(x)$ is a solution to the differential equation $y''-2xy'+2ny=0$, we have $H_n(x)=0$ for all x; but this is impossible. ■

Let us return to the proof of the proposition. Suppose that $\mathbf{q}\neq 0$; without loss of generality we can assume $q_2\neq 0$. Since $H_1(x)=0$ only for $x=0$, and $H_0(x)\neq 0$ for all x, we have $\lambda_0,\lambda_1\in\sigma(\mathbf{q})$. Let $n>1$. Suppose that $\Phi_{n-1,1,0}(\mathbf{q})=0$, then according to Lemma 6, $\Phi_{n,0,0}(\mathbf{q})\neq 0$. ■

Using Proposition 3 we can give the complete description of the spectrum $H_\alpha(\mathbf{q})$ in the case of an isotropic H^0. Moreover, in this case the explicit form of the Green function $G^0(\mathbf{x},\mathbf{x}';\zeta)$ is known, and therefore, we can give the explicit form of the Krein $\mathcal{Q}$-function and eigenfunction of $H_\alpha(\mathbf{q})$. In particular, the equation for the point perturbation levels $E_n(\mathbf{q})$ can be obtained in an explicit form. The mentioned Green function has the form[18]

$$G^0(\mathbf{x},\mathbf{y};\zeta)=-\frac{1}{2(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\left[\frac{U(-\zeta;\xi)U'(-\zeta;-\eta)+U'(-\zeta;\xi)U(-\zeta;-\eta)}{|\mathbf{x}-\mathbf{y}|}\right.$$
$$\left.+\frac{U(-\zeta;\xi)U'(-\zeta;-\eta)-U'(-\zeta;\xi)U(-\zeta;-\eta)}{|\mathbf{x}+\mathbf{y}|}\right], \tag{16}$$

where $\xi=(|\mathbf{x}+\mathbf{y}|+|\mathbf{x}-\mathbf{y}|)/2$, $\eta=(|\mathbf{x}+\mathbf{y}|-|\mathbf{x}-\mathbf{y}|)/2$, $U(\nu;z)$ is the parabolic cylinder function[44] (in the Whittaker notation $U(\nu;z)=D_{-\nu-1/2}(z)$), and U' denotes the derivative of U with respect to the second argument

$$U'(\zeta;y)=\frac{\partial}{\partial y}U(\zeta;y)\,.$$

Using (16), we get the following expression for the Q-function:

$$Q(\zeta;\mathbf{q})=-\frac{1}{8(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\Bigg[(q^2-4\zeta)U(-\zeta,q)U(-\zeta,-q)+4U'(-\zeta,q)U'(-\zeta,-q)$$
$$-\frac{2}{q}(U'(-\zeta,q)U(-\zeta,-q)-U(-\zeta,q)U'(-\zeta,-q))\Bigg], \tag{17}$$

where $q=|\mathbf{q}|$. Due to the symmetry of the problem, the $\mathcal{Q}$-function depends on q only, so we shall write often $Q(\zeta;q)$ instead of $Q(\zeta;\mathbf{q})$. Introducing the notation $\mathcal{U}(\zeta;y)=U(\zeta;y)U(\zeta;-y)$, we can rewrite (17) in the sometimes more useful form

$$Q(\zeta;\mathbf{q})=-\frac{1}{4(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\left[(q^2-4\zeta)\mathcal{U}(-\zeta;q)-\frac{1}{q}\mathcal{U}'(-\zeta;q)-\mathcal{U}''(-\zeta;q)\right], \tag{18}$$

where the prime denotes the derivative with respect to the second argument as before. Passing to limit we get at $q=0$

$$Q(\zeta;0)=-\frac{1}{\sqrt{8}\pi}\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}. \tag{19}$$

It is interesting to compare (19) with the Krein $\mathcal{Q}$-function $Q^{(1)}(\zeta;0)$ for the one-dimensional harmonic oscillator:[26]

$$Q^{(1)}(\zeta;0)=2^{-3/2}\frac{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}.$$

Curiously, in the case of the free Hamiltonian $H^0=-\Delta$, the $\mathcal{Q}$-functions Q_d for $d=1$ and for $d=3$ are also related as follows:

$$Q_1^{-1}(\zeta)=-8\pi Q_3(\zeta)\,. \tag{20}$$

Namely, for the free Hamiltonian $Q_1(\zeta)=(2\sqrt{-\zeta})^{-1}$, $Q_3(\zeta)=-(4\pi)^{-1}\sqrt{-\zeta}$. For $q\neq 0$ relation (20) for $\mathcal{Q}$-functions of the harmonic oscillators is violated.

It is useful to consider the behavior of the function $\zeta\mapsto Q(\zeta;q)$ near the singular points, i.e., near the poles and in a neighborhood of $-\infty$. Using properties of the parabolic cylinder functions,[43] we have

$$Q(\zeta;0)=-\frac{(2n+1)!!}{(2\pi)^{3/2}(2n)!!}\left(\frac{1}{\zeta-\lambda_{2n}}-\ln 2+1-\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k(1+2k)}+O(\zeta-\lambda_{2n})\right),$$

as $\zeta\to\lambda_{2n}$. If $\mathbf{q}\neq 0$, the coefficients for corresponding asymptotics are cumbrous enough, and we give the leading term only:

$$Q(\zeta;q) = -\frac{\exp(-q^2/2)}{(2\pi)^{3/2}2^{n+2}n!}(2(n+1)H_n^2(q/\sqrt{2}) + \sqrt{2}(q^{-1}-q)H_n(q/\sqrt{2})H_{n+1}(q/\sqrt{2}) + H_{n+1}^2(q/\sqrt{2}))(\zeta-\lambda_n)^{-1} + O(1), \tag{21}$$

as $\zeta \to \lambda_n$.

For $\operatorname{Re}\zeta \to -\infty$, we have

$$Q(\zeta;q) = -\frac{\sqrt{-\zeta}}{4\pi}\left(1 - \frac{q^2}{8}\zeta^{-1} + \frac{8-q^4}{128}\zeta^{-2} + O(\zeta^{-3})\right). \tag{22}$$

It is important to note that the leading term in (22) coincides with the Krein Q-function for the free Hamiltonian $-\Delta$.

Now consider the properties of the function $q \mapsto Q(\zeta;q)$. Since $U(\nu;z)$ is an entire function of z, the function $q \mapsto Q(\zeta;q)$ at $\zeta \notin \operatorname{spec}(H^0)$ can be extended to a real analytic even function on $\mathbb{R}$ [see (18)]. In particular,

$$\frac{\partial}{\partial q} Q(\zeta;0) = 0.$$

As to the second derivative, we can obtain after some algebra

$$\frac{\partial^2}{\partial q^2} Q(\zeta;0) = \frac{1}{8\sqrt{6}\pi}\left[(4\zeta^2+1)\frac{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)} - 8\zeta\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}\right]. \tag{23}$$

For the fixed $\zeta \in \mathbb{R}\setminus\operatorname{spec}(H^0)$, the asymptotics of Q at $q \to \infty$ is given by

$$Q(\zeta;q) = -\frac{1}{8\pi}\left[q - \frac{2\zeta}{q} - \frac{1+2\zeta^2}{q^3} + O\left(\frac{1}{q^5}\right)\right]. \tag{24}$$

This follows from the asymptotics for $\mathcal{U}(\zeta;q)$ at $q \to \infty$:[45]

$$\mathcal{U}(\zeta;q) = \frac{\sqrt{2\pi}}{\Gamma\left(\frac{1}{2}+\zeta\right)}\left[\frac{1}{X} + O\left(\frac{1}{X^5}\right)\right],$$

where $X = \sqrt{q^2+4\zeta}$.

Further the following formula will be also useful

$$\frac{\partial Q}{\partial \zeta}(\zeta;0) = \frac{1}{4\sqrt{2}\pi}\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)} G\left(\frac{1}{2}-\zeta\right). \tag{25}$$

Here and below we use the standard notations[43]

$$G(z) = \psi\left(\frac{z}{2}+\frac{1}{2}\right) - \psi\left(\frac{z}{2}\right); \qquad \psi(z) = \frac{\Gamma'(z)}{\Gamma(z)}.$$

The plot of the graphs for the function $Q(\zeta;q)$ is shown in Figs. 1 and 2.

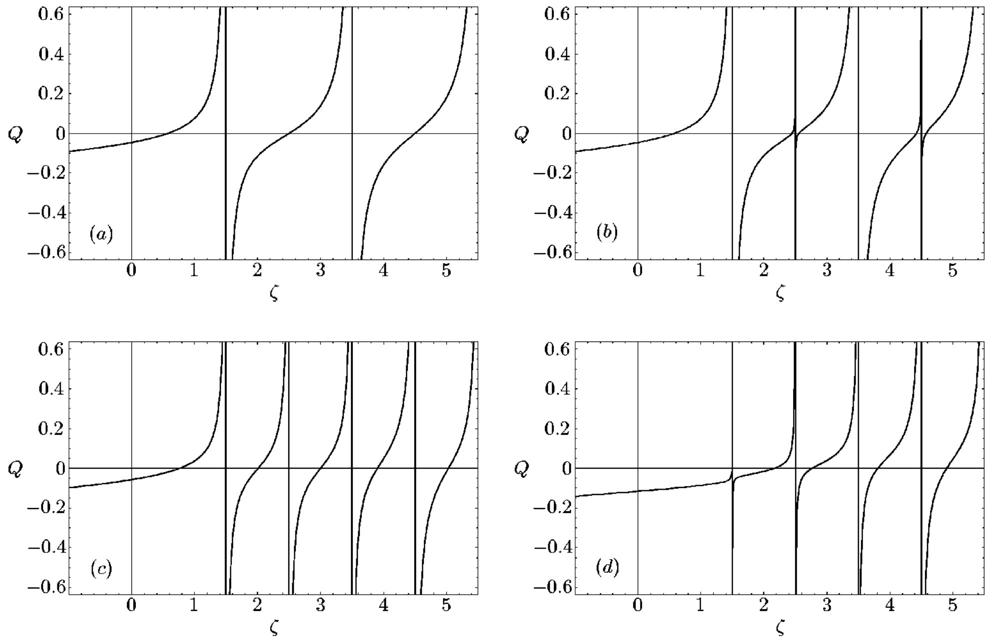

FIG. 1. Q as a function of ζ for (a) $q=0$, (b) $q=1/10$, (c) $q=1$, (d) $q=3$.

In the case of an isotropic oscillator, the functions $E_n(\mathbf{q})$ depend only on q and we will denote them by $E_n(q)$. Further properties of these functions [and, in particular, of the spectrum of $H_\alpha(\mathbf{q})$] for the isotropic case are given in Theorem 3 below, which is one of the main results of the article.

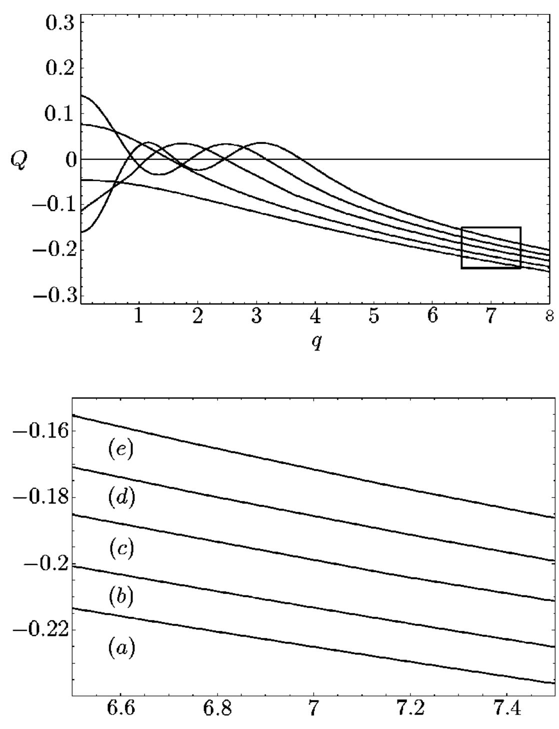

FIG. 2. Q as a function of q for (a) $\zeta=0$, (b) $\zeta=1$, (c) $\zeta=2$, (d) $\zeta=3$, (e) $\zeta=4$.

Theorem 3: *The following assertions take place.*

(1) The functions $E_n(q)$, $n\in\mathbb{N}$ are real-analytic. If $\alpha=0$ and $n>0$, then in a vicinity of zero, these functions are continuous branches of a two-valued analytic function.

(2a) $E_0(0)<\lambda_0$ for each α, $\alpha\in\mathbb{R}$.

(2b) If $\alpha>0$, then $E_{2n+1}(0)=\lambda_{2n+1}$ and $\lambda_{2n+1}<E_{2n+2}(0)<\lambda_{2n+2}\forall n\in\mathbb{N}$.

(2c) If $\alpha<0$, then $\lambda_{2n}<E_{2n+1}(0)<\lambda_{2n+2}$ and $E_{2n+2}(0)=\lambda_{2n+2}\forall n\in\mathbb{N}$.

(2d) If $\alpha=0$, then $E_{2n+1}(0)=E_{2n+2}(0)=\lambda_{2n+1}\forall n\in\mathbb{N}$.

(3a) If $\alpha\neq 0$, then for any $n>0$

$$\frac{\partial E_n}{\partial q}(0)=0\,. \tag{26}$$

If $n=0$, then (26) is valid for any α.

(3b) *If $\alpha>0$ (respectively, $\alpha<0$), then*

$$\frac{\partial^2 E_n}{\partial q^2}(0)=\frac{1}{8\sqrt{6}G\left(\frac{1}{2}-E_n(0)\right)}\left(\frac{4E_n^2(0)+1}{8\pi^2\alpha^2}-8E_n(0)\right), \tag{27}$$

for any even (respectively, odd) n. If $n=0$, then (27) is valid for any α.

(3c) *If $\alpha=0$, then $(\partial E_{2n+1}/\partial q)(0)<0$, $(\partial E_{2n+2}/\partial q)(0)>0$, and $(|(\partial E_{2n+1}/\partial q)(0)| =|(\partial E_{2n+2}/\partial q)(0)|\forall n\in\mathbb{N}$.*

(4) *If $q\neq 0$, then $\lambda_{n-1}<E_n(q)<\lambda_n\forall n\in\mathbb{N}$.*

(5) $\lim_{q\to\infty}E_n(q)=\lambda_n\forall n\in\mathbb{N}$.

Proof: Item (4) follows immediately from Proposition 3 and the definition of the functions E_n. Formula (19) shows that $Q(\zeta;0)=0$ if and only if $\zeta=\lambda_{2n+1}$ for some $n\in\mathbb{N}$; therefore, items (2a)–(2d) follow from Theorem 2. Using the standard version of the implicit function theorem and the Proposition 3 again, we see that $E_n(q)$ are real analytic at $q>0$. Moreover, item (3) of Theorem 2 implies that (i) $E_n(q)$ are real-analytic at $q=0$ for even n if $\alpha>0$, (ii) $E_n(q)$ are real-analytic at $q=0$ for odd n if $\alpha<0$, and (iii) $E_0(q)$ is real-analytic at $q=0$ for any α. In all these cases, the derivatives of E_n can be found from the equations

$$\frac{\partial Q}{\partial\zeta}\frac{\partial E_n}{\partial q}+\frac{\partial Q}{\partial q}=0\,,$$

$$\frac{\partial Q}{\partial\zeta}\frac{\partial^2 E_n}{\partial q^2}+\frac{\partial^2 Q}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+2\frac{\partial^2 Q}{\partial\zeta\partial q}\frac{\partial E_n}{\partial q}+\frac{\partial^2 Q}{\partial q^2}=0. \tag{28}$$

Since $(\partial Q/\partial q)(E;0)=0$ if $E\notin\operatorname{spec}(H^0)$, equation (26) follows from (28) in the considered cases. In virtue of (26), the second derivative of E_n is given by

$$\frac{\partial^2 E_n}{\partial q^2}(0)=-\frac{\partial^2 Q}{\partial q^2}\left(\frac{\partial Q}{\partial\zeta}\right)^{-1}(E_n(0);0). \tag{29}$$

Substituting (23) and (25) into (29) and using (9) we get (27).

Now consider the singular case when $E_n(0)$, $n\geqslant 1$, coincides with a point of the form λ_{2m+1}. In a neighborhood of the point $(E_n(0),0)$, introduce the function

$$\tilde{Q}_\alpha(\zeta;q)=\frac{Q(\zeta;q)-\alpha}{\Gamma\left(\frac{1}{2}-\zeta\right)},$$

which is smooth with respect to (ζ,q) and analytic with respect to the first argument ζ. In a vicinity of $(E_n(0),0)$ we have

$$\tilde{Q}_\alpha(E_n(q);q)=0\,. \tag{30}$$

Further,

$$\frac{\partial\tilde{Q}_\alpha}{\partial\zeta}=\frac{1}{\Gamma(1/2-\zeta)}\,\frac{\partial Q}{\partial\zeta}+(Q-\alpha)\,\frac{\Gamma'(1/2-\zeta)}{\Gamma^2(1/2-\zeta)}. \tag{31}$$

Since $(\partial Q/\partial\zeta)(\zeta;0)$ is a finite number at $\zeta=\lambda_{2m+1}$ and $\Gamma(1/2-\zeta)$ has a pole at λ_{2m+1}, the first term in (31) vanishes at the point $(\lambda_{2m+1},0)$. The value of the function $\Gamma'(1/2-\zeta)/\Gamma^2(1/2-\zeta)$ at $\zeta=\lambda_{2m+1}$ is a nonzero finite number. Finally, $Q(\lambda_{2m+1},0)=0$; thus $\partial\tilde{Q}_\alpha/\partial q$ vanishes at the point λ_{2m+1} if and only if $\alpha=0$. Therefore, if $\alpha\neq0$, then each function $E_n(q)$ has an analytic continuation in a neighborhood of the point $q=0$. Since $q\mapsto\tilde{Q}_\alpha(\lambda_{2m+1};q)$ is an even function, we get easily (26).

Let now $\alpha=0$. Then

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}=\frac{1}{\Gamma(1/2-\zeta)}\,\frac{\partial^2 Q}{\partial\zeta^2}+2\,\frac{\Gamma'(1/2-\zeta)}{\Gamma^2(1/2-\zeta)}\,\frac{\partial Q}{\partial\zeta}-Q\,\frac{\Gamma''(1/2-\zeta)\Gamma(1/2-\zeta)-2\Gamma'^2(1/2-\zeta)}{\Gamma^3(1/2-\zeta)}. \tag{32}$$

It is easy to see that the first and last terms in (32) vanishes at the point $(\lambda_{2m+1},0)$, whereas the second one does not. Therefore, $\partial^2\tilde{Q}_0/\partial\zeta^2\neq0$ at the point $(\lambda_{2m+1},0)$, and $E_n(q)$ being solutions of (30), are continuous branches a two-valued analytic function in a vicinity of $(\lambda_{2m+1},0)$. Obviously, at the point $(\lambda_{2m+1},0)$ the following relation is valid

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+2\,\frac{\partial^2\tilde{Q}_0}{\partial\zeta\partial q}\,\frac{\partial E_n}{\partial q}+\frac{\partial\tilde{Q}_0}{\partial\zeta}\,\frac{\partial^2 E_n}{\partial q^2}+\frac{\partial^2\tilde{Q}_0}{\partial q^2}=0\,.$$

Since $\partial\tilde{Q}_0/\partial\zeta=0$ at the considered point, we get the quadratic equation for $\partial E_n/\partial q$:

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+\frac{\partial^2\tilde{Q}_0}{\partial q^2}=0\,.$$

As a result, we complete the proof of items (1) and (3c). It remains to prove (5). Fix $n\in\mathbb{N}$ and let ε, $0<\varepsilon<1$, is given. According to (24) we can choose $q_0>0$ such that $Q(\lambda_n-\varepsilon;q)-\alpha<0$ if $q\geqslant q_0$. Since $Q(E_n(q);q)-\alpha=0$ and the function $E\mapsto Q(E;q)$ increases in the interval $\lambda_{n-1}<E<\lambda_n$, we have $E_n(q)>\lambda_n-\varepsilon$ as $q\geqslant q_0$. Moreover, $E_n(q)<\lambda_n$, and the proof is completed. ■

The structure of spec$(H_\alpha(q))$ given by Theorem 3 is presented in Table I. The peculiarities of this table at $q=0$ can be understood from the point of view the symmetry group of the problem. It is well known that for a generic spherically symmetric potential $V(\mathbf{r})$, the eigenvalues λ of the operator $H^0=-\Delta+V$ are parametrized by three quantum numbers: $\lambda=\lambda_{n_r,l,m}$, where n_r ($n_r=0,1,\ldots$) is the so called principal (or total) quantum number; l ($l=0,1,\ldots$) is the orbital quantum number, and m ($m=-l,-l+1,\ldots,l-1,l$) is the magnetic quantum number. Each eigenvalue $\lambda_{n_r,l,m}$ is degenerate with multiplicity $2l+1$, namely, $\lambda_{n_r,l,m}=\lambda_{n_r,l,m'}$ if $m,m'\in\{-l,-l+1,\ldots,l-1,l\}$. This degeneracy is related to the invariance of H^0 with respect to the rotation group $\mathbb{SO}(3)$: eigensubspaces of H^0 carry an irreducible representation of this group. In general, $\lambda_{n_r,l,m}\neq\lambda_{n'_r,l',m'}$ if $n_r\neq n'_r$ or $l\neq l'$. The eigenvalues of an isotropic harmonic oscillator have an additional (so-called accidental) degeneracy: Each eigensubspace L_n is decomposed on the sub-

TABLE I. The structure of spec($H_\alpha(q)$).

	$q=0$	$q\neq 0$
$\alpha>0$	$\sigma_1=\{E_{2n}(0):\, n\in\mathbb{N}\}$	$\sigma_1=\{E_n(q):\, n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}:\, n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}:\, n\in\mathbb{N}\}$
	$\sigma_3=\{\lambda_{2n+1}:\, n\in\mathbb{N}\}$	$\sigma_3=\varnothing$
	$\sigma_4=\varnothing$	$\sigma_4=\varnothing$
$\alpha=0$	$\sigma_1=\{1/2\}$	$\sigma_1=\{E_n(q):\, n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}:\, n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}:\, n\in\mathbb{N}\}$
	$\sigma_3=\varnothing$	$\sigma_3=\varnothing$
	$\sigma_4=\{\lambda_{2n+1}:\, n\in\mathbb{N}\}$	$\sigma_4=\varnothing$
$\alpha<0$	$\sigma_1=\{E_{2n+1}(0):\, n\in\mathbb{N}\}\cup\{E_0(0)\}$	$\sigma_1=\{E_n(q):\, n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}:\, n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}:\, n\in\mathbb{N}\}$
	$\sigma_3=\{\lambda_{2n+1}:\, n\in\mathbb{N}\}$	$\sigma_3=\varnothing$
	$\sigma_4=\varnothing$	$\sigma_4=\varnothing$

spaces $L_n^{(l)}$ with angular momentum $l=n,n-2,\ldots,0$ (if n is even) or $l=n,n-2,\ldots,1$ (if n is odd). This accidental degeneracy is related to the invariance of the Hamiltonian H^0 of an isotropic harmonic oscillator with respect to the group $\mathbb{U}(3)$. Indeed,

$$H^0=\sum_{j=1}^{3} a_j^+ a_j+\tfrac{3}{2},$$

where a_j^+ and a_j are standard creation and annihilation operators.[41] Therefore, H^0 is invariant with respect to the transformation

$$a_j\to a_j'=\sum_{j=1}^{3} u_{kj}a_j\,,\qquad a_j^+\to a'^+_j=\sum_{j=1}^{3} u_{kj}^* a_j^+\,,$$

where (u_{jk}) is a unitary matrix. If $q=0$, then $H_\alpha(0)$ is a spherically symmetric perturbation of H^0 that violates the $\mathbb{U}(3)$-symmetry. To prove this, we note that operators $a_j^+a_k$ are generators of the Lie group $\mathfrak{u}(3)$. Therefore, if $H_\alpha(0)$ is invariant with respect to the considered representation of $\mathbb{U}(3)$, we must have $[H_\alpha(0),H^0]=0$. On the other hand it is easy to show that for $\zeta\in\mathbb{C}\setminus\mathbb{R}$ the operator $[R_\alpha(\zeta),R^0(\zeta)]$ has a nonzero integral kernel.

Since point perturbations cannot change states with nonzero angular momentum l (see, e.g., 8), the part σ_2 (at $q=0$) may contain only even eigenvalues λ_{2n} and we see this in Table I. Since all states from L_n have the same parity $(-1)^n$, the isotropic oscillator has no stationary states with a nonzero dipole momentum.[35] On the other hand every eigensubspace of $H_0(0)$ with eigenvalue from σ_4 have an eigenfunction with $l=0$ (this is the eigenfunction from item 4 of Theorem 1). Therefore, point perturbations of an isotropic harmonic oscillator can lead to an appearance of eigenstates with nonzero dipole momentum.

An alternative tool to understand the energy degeneracy of the three-dimensional isotropic oscillator gives the supersymmetry theory.[46–48] We will not dwell here on this approach, nevertheless note that the analysis performed in the cited papers requires a modification in the s-channel only.

The functions E_n depend not only on the position parameter q, but also on the strength α; we will denote these dependencies as $E_n=E_n(q,\alpha)$. If $E(q,\alpha_0)$ coincides with one of the numbers $\mathcal{E}_m$, then in a vicinity of α_0, the function $\alpha\mapsto E_n(q,\alpha)$ is a continuous branch of the inverse function to $E\mapsto Q(E;q)$. It is already known from Proposition 1 that the following limits take place:

$$\lim_{\alpha\to+\infty} E_n(q;\alpha)=\lambda_n\,,\qquad \lim_{\alpha\to-\infty} E_n(q;\alpha)=\lambda_{n-1}\,,$$

where $\lambda_{-1}=-\infty$. Now we make more precise this behavior. From (22) we get the asymptotics of the function $E_0(q;\alpha)$ for the fixed $q\geqslant 0$ as $\alpha\rightarrow-\infty$,

$$E_0(q;\alpha)=-16\pi^2\alpha^2+\frac{q^2}{4}+\frac{1}{128\pi^2\alpha^2}+O\left(\frac{1}{\alpha^4}\right), \tag{33}$$

or in terms of the point perturbation of the initial operator (1)

$$E_0(q;\alpha)=-\frac{\hbar^2}{2\mu l_s^2}+\frac{\mu\Omega^2q^2}{2}+\frac{\mu\Omega^2 l_s^2}{4}+O(l_s^4), \tag{34}$$

where the scattering length l_s tends to 0. Expression (34) means that up to the infinitely small term $O(l_s^2)$ the ground state of $\hat{H}_\alpha(\mathbf{q})$ equals to the ground state of the point perturbation of the free Hamiltonian $-\hbar^2\Delta/2\mu$ with the same scattering length l_s shifted by the potential $V(\mathbf{r})=\mu\Omega^2\mathbf{r}^2/2$ at the point $\mathbf{r}=\mathbf{q}$. Equation (34) shows that at least for the isotropic harmonic oscillator its potential can be recovered from the dependence of the ground state of the point perturbation on the position of the potential support. It is reasonable to suppose that this is true for more general forms of the potential V; we consider this conjecture elsewhere.

Now consider the behavior of $E_n(q;\alpha)$ in a vicinity of the poles of $Q(\zeta,q)$. We start with the general case $q\neq 0$. Using (21) we get as $\alpha\rightarrow\pm\infty$

$$\begin{aligned}E_n(q;\alpha)=\lambda_n^{\pm}-\frac{\exp(-q^2/2)}{(2\pi)^{3/2}2^{n+2}n!}&(2(n+1)H_n^2(q/\sqrt{2})+\sqrt{2}(q^{-1}-q)H_n(q/\sqrt{2})H_{n+1}(q/\sqrt{2})\\&+H_{n+1}^2(q/\sqrt{2}))\alpha^{-1}+O(\alpha^{-2}),\end{aligned} \tag{35}$$

where $\lambda_n^+=\lambda_n$ and $n\geqslant 0$ as $\alpha\rightarrow+\infty$, and $\lambda_n^-=\lambda_{n-1}$ and $n\geqslant 1$ as $\alpha\rightarrow-\infty$.

In the case $q=0$, we are in position to give a compact form for more precise asymptotics of $E_n(q;\alpha)$. Denote

$$\Lambda_n(\alpha)=\frac{(2n+1)!!}{(2\pi)^{3/2}(2n)!!}\alpha^{-1}-\left(\frac{(2n+1)!!}{(2\pi)^{3/4}(2n)!!}\right)^2\left(\ln 2-1+\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k(1+2k)}\right)\alpha^{-2}.$$

For eigenvalues with even indices we have

$$E_{2n}(0;\alpha)=\begin{cases}\lambda_{2n-1} & \text{for } \alpha\leqslant 0 \text{ and } n\geqslant 1\\ -16\pi^2\alpha^2+\dfrac{1}{128\pi^2}\alpha^{-2}+O(\alpha^{-4}) & \text{for } \alpha\rightarrow-\infty \text{ and } n=0\\ \lambda_{2n}-\Lambda_n(\alpha)+O(\alpha^{-3}) & \text{for } \alpha\rightarrow+\infty \text{ and } n\geqslant 0.\end{cases} \tag{36}$$

For the odd indices

$$E_{2n+1}(0;\alpha)=\begin{cases}\lambda_{2n+1} & \text{for } \alpha\geqslant 0\\ \lambda_{2n}-\Lambda_n(\alpha)+O(\alpha^{-3}) & \text{for } \alpha\rightarrow-\infty.\end{cases} \tag{37}$$

Formulas (35)–(37) explain peculiarities in the plots of functions E_n on Figs. 3 and 4. Note that in Eqs. (33)–(37) the remainder terms depend on n.

The isotropic harmonic oscillator has an equidistant spectrum. After the perturbation by a zero-range potential, the distances between energy levels are changed and become dependent on the energy index n. This is important in the connection with the problem of the controlled modulation of the binding energy of the impurity center in quantum dots, that can be used to design nonlinear opto-electronic active elements.[6] The asymptotic formulas (34)–(37) give very accurate expressions for the excited energies in the most interesting case of a deep zero-range well

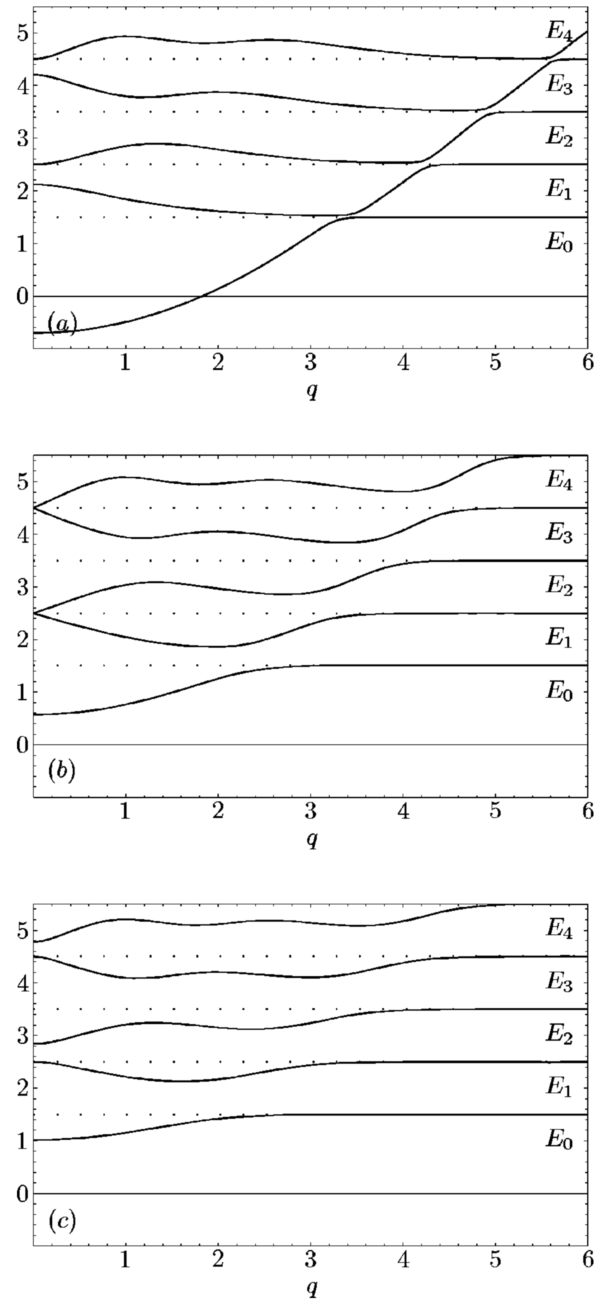

FIG. 3. E_n as a function of q for (a) $\alpha=-\alpha^0$, (b) $\alpha=0$, (c) $\alpha=\alpha^0$.

$(\alpha\to-\infty)$ as well as for the case of a shallow well $(\alpha\to+\infty)$, which confirm numerical results from Ref. 6. Note also that Proposition 1 and Theorem 3 imply a remarkable distinction between the excited energy for the ground state and that for the other ones: The energy $E_1(q;\alpha)-E_0(q;\alpha)$ can take an arbitrary value depending on q and α; on the other hand, energies $\lambda_n-E_n(q;\alpha)$ and $E_{n+1}(q;\alpha)-\lambda_n(n\geqslant 1)$ are bounded by 1. Since at fixed α, $\alpha\ll-1$, the function $q\mapsto E_1(q;\alpha)-E_0(q;\alpha)$ is injective for moderate values of q, the position of an impurity in the quantum dot may be determined from the spectroscopy data.

We show the plot of the energies $E_1(q;\alpha)-E_0(q;\alpha)$ and $\lambda_1-E_1(q;\alpha)$ as functions of q and α on Figs. 5 and 6, respectively.

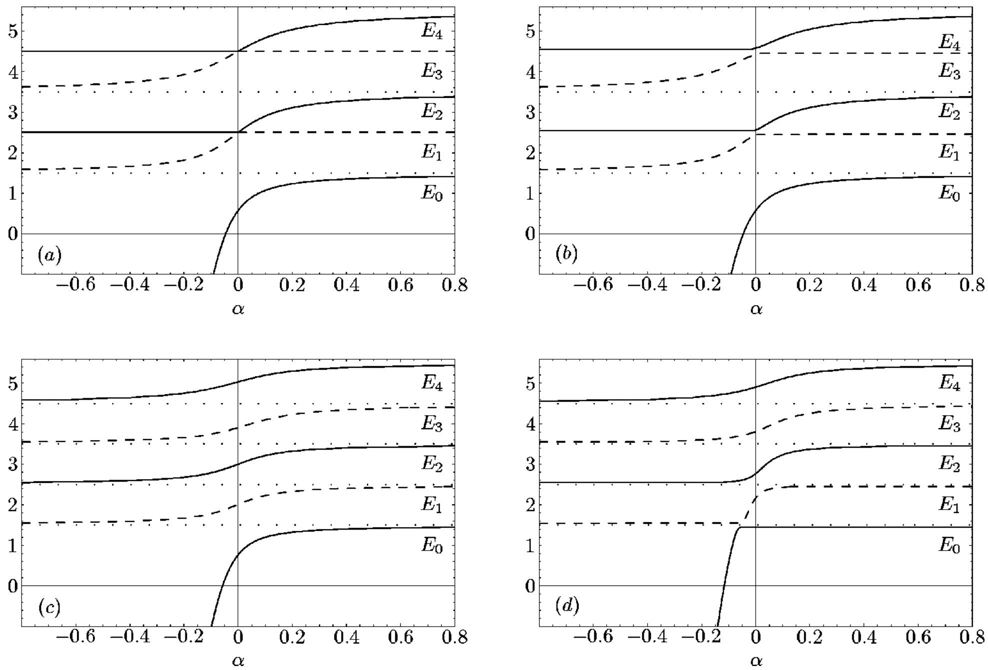

FIG. 4. E_n as a function of α for (a) $q=0$, (b) $q=1/10$, (c) $q=1$, (d) $q=3$.

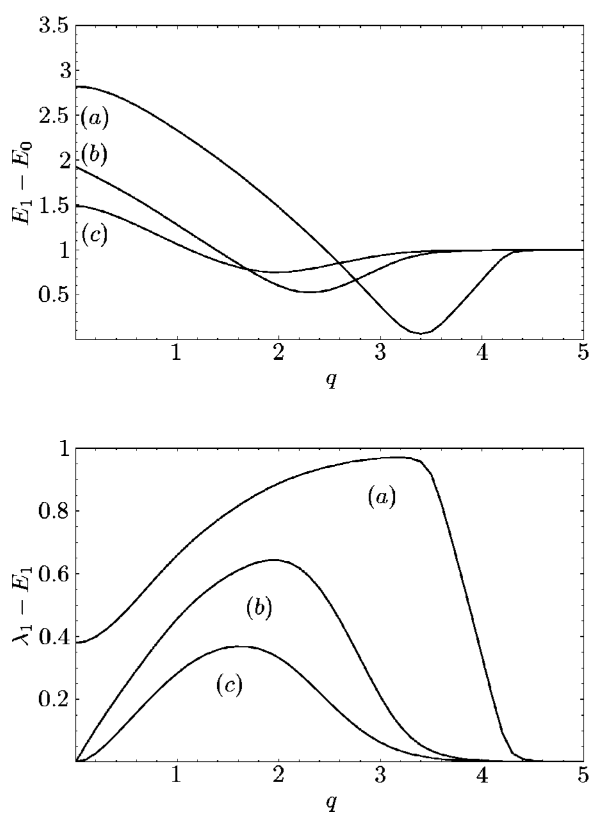

FIG. 5. The exciting energy as a function of q for (a) $\alpha=-\alpha^0$, (b) $\alpha=0$, (c) $\alpha=\alpha^0$.

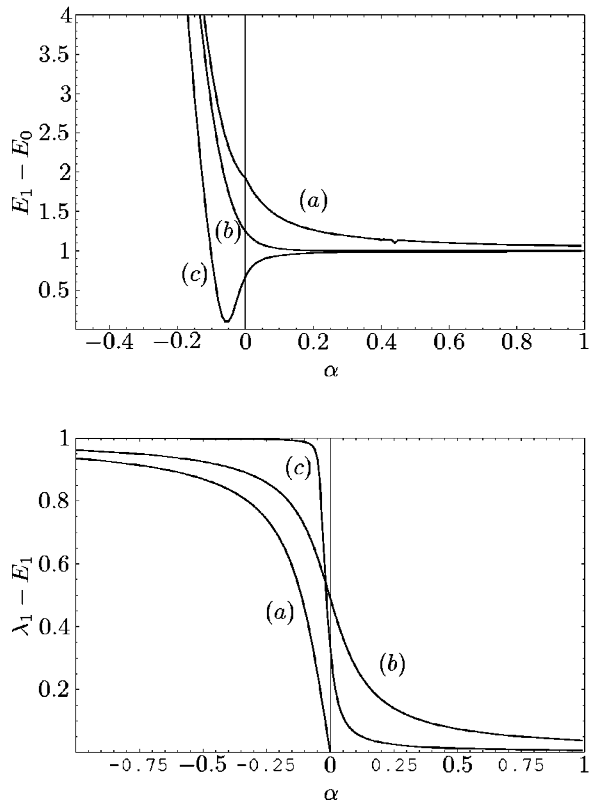

FIG. 6. The exciting energy as a function of α for (a) $q=0$, (b) $q=1$, (c) $q=3$.

In conclusion we give the following remark. Let $q\colon [0,\infty)\to\mathbb{R}$ be a smooth function obeying the conditions

(H1) $q\geqslant 0$ and the function $r\mapsto q(r)+r^2/4$ is nondecreasing;
(H2) $q'(r)\leqslant 0$, and let κ_0 and κ_1 be the first two eigenvalues of the operator $H^0+q=-\Delta+r^2/4+q(r)$. It is proven in Ref. 49 that $\kappa_0/\kappa_1<\lambda_0/\lambda_1$, if $q\neq 0$. Using Theorems 3 and A it is easy to construct smooth functions q with properties (H1) and
(H2a) $q'(r)\geqslant 0$, such that $\kappa_0/\kappa_1>\lambda_0/\lambda_1$.

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