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# A modification of the Bohr-Sommerfeld quantization condition 

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#### Abstract

The Bohr-Sommerfeld quasiclassical quantization condition for a central potential is modified in such a way that the constant $\gamma$ becomes dependent on the angular momentum $l$ and on the potential behaviour at small distances. This form of the quantization condition is especially simple in the case $l=0$. When applied to some particular potentials, taken as examples, the present approximation provides more accurate values of the level energies than the conventional form of the quantization condition. Application of the quasiclassical approach to singular potentials with 'collapse' and to the superstrong Coulomb field induced by a charge $Z>137$ is also considered.


## 1. Introduction

The well known quantization condition for a one-dimensional potential problem is

$$
\int_{x_{1}}^{x_{2}}[2 m(E-V(x))]^{1 / 2} \mathrm{~d} x=(n+\gamma) \pi \hbar
$$

where $x_{1}$ and $x_{2}$ are the classical turning points and $\gamma=\frac{1}{2}$. In the case of a threedimensional central potential the origin, $r=0$, is a singularity. The conventional approach (Kramers 1926, Langer 1937; see also Landau and Lifshitz 1963, Berry and Mount 1972) is to substitute $l(l+1)$ by $\left(l+\frac{1}{2}\right)^{2}$ in the centrifugal part of the kinetic energy, conserving the value of $\gamma=\frac{1}{2}$. This 'Langer's correction' is widely used in applications of the quasiclassical approach to calculation of energy levels as well as to scattering problems (Berry and Mount 1972, see also recent papers by Delos and Carlson 1975, Sukumar and Bardsley 1975). In a previous work (Marinov and Popov 1974) we proposed to omit the centrifugal energy in the effective momentum $p(r)$, changing the constant $\gamma$ correspondingly. For an important class of potentials-those with a power singularity at $r \rightarrow 0, V(r) \sim r^{-\alpha}(0 \leqslant \alpha<2)$, and decreasing as an exponential at infinity -the proposed quantization condition at $l=0$ has a form analogous to the onedimensional case,

$$
\begin{equation*}
\int_{0}^{r_{0}}[2 m(E-V(r))]^{1 / 2} \mathrm{~d} r=\left(n_{r}+\gamma\right) \pi \hbar, \quad \gamma=\frac{3-\alpha}{2(2-\alpha)} . \tag{1.1}
\end{equation*}
$$

Here $V\left(r_{0}\right)=E, n_{r}=0,1,2, \ldots$ is the radial quantum number (the subscript $r$ will be omitted in the following).

Using dimensionless variables $\lambda, g, x$ (with atomic units $m=\hbar=1$ ) and the function $Q(z)$,

$$
\begin{align*}
& E=-\frac{\lambda^{2}}{2 m R^{2}}, \quad V(r)=-\frac{g^{2} v(x)}{2 m R^{2}} \\
& x=r / R, \quad v(x) \geqslant 0  \tag{1.2}\\
& Q(z)=\int_{0}^{x_{0}}\left(v(x)-z^{2}\right)^{1 / 2} \mathrm{~d} x
\end{align*}
$$

equation (1.1) may be reduced to the form

$$
\begin{equation*}
g Q(\lambda / g)=(n+\gamma) \pi \tag{1.3}
\end{equation*}
$$

which is much simpler than the conventional condition. The notations used are as follows : $R$ is the range of the potential $V, g$ is the strength (coupling) constant, $v(x)$ is the potential form function, and $x_{0}=x_{0}(z)$ is the root of the equation $v(x)=z^{2}$.

The function $Q(z)$ may be calculated analytically for some interesting potentials. For instance, in the case $v(x)=\exp (-x), \alpha=0, Q(z)=2\left[\left(1-z^{2}\right)^{1 / 2}-z \cos ^{-1} z\right]$ at $0 \leqslant z<1$. The approximate equation (1.3) for the energy takes the form

$$
\begin{equation*}
\left(g^{2}-\lambda^{2}\right)^{1 / 2}-\lambda \cos ^{-1} \lambda / g=\left(n+\frac{3}{4}\right) \pi / 2 \tag{1.4}
\end{equation*}
$$

Note that the Schrödinger equation for this potential may be solved explicitly at $l=0$, and the exact equation is

$$
\begin{equation*}
\mathrm{J}_{2 \lambda}(2 g)=0 \tag{1.5}
\end{equation*}
$$

The equation (1.4) is obtained from (1.5) using the Debye asymptotics of the Bessel function (see Jahnke et al 1960):

$$
\mathrm{J}_{v}(v / \cos \beta) \simeq(2 / v \pi \tan \beta)^{1 / 2} \cos [v(\tan \beta-\beta)-\pi / 4] .
$$

This formula is known to be rather accurate.
For some potentials used in atomic and nuclear physics the quantization condition (1.1) allows one to calculate easily the level energies with reasonable accuracy; the error is no more than a few per cent, even for the ground state. However, this fact was shown in our previous work only for the s states $(l=0)$. The purpose of the present work is to generalize the approach to the case of arbitrary values of $l$, as well as to apply the method to singular potentials with a 'collapse'.

## 2. Deduction of the quantization condition

Consider the Schrödinger equation for the radial wavefunction $\chi(x), x=r / R$ :

$$
\begin{equation*}
\chi^{\prime \prime}+\left[g^{2} v(x)-l(l+1) x^{-2}-\lambda^{2}\right] \chi=0 \tag{2.1}
\end{equation*}
$$

Assume that $v(x) \sim x^{-\alpha}$ when $x \rightarrow 0$. The centrifugal energy is dominating at $x \ll x_{1}=\left[l(l+1) / g^{2}\right]^{1 /(2-\alpha)}$ while the potential term $g^{2} v(x)$ dominates at $x_{1} \ll x \ll(g / \lambda)^{2 / \alpha}$. In the region of small $x$ we put $v(x)=x^{-x}$, omit the term $-\lambda^{2}$ and solve the equation exactly:

$$
\begin{align*}
& \chi=C x^{1 / 2} \mathrm{~J}_{v}\left(k x^{\beta}\right), \quad v=(2 l+1) /(2-\alpha), \\
& k=g / \beta, \quad \beta=1-\alpha / 2 . \tag{2.2}
\end{align*}
$$

The $n$th energy level occurs at sufficiently large $g$, ie $g>g_{n l} \sim n \pi a, a=\int_{0}^{\infty} v^{1 / 2} \mathrm{~d} x$, so that at high $n$ there exists a region of small $x$ where the asymptotics of the Bessel function may be used, $k x^{\beta} \gg 1$. Thus

$$
\begin{align*}
& \chi(r) \simeq C r^{\alpha / 4} \sin \theta(r)  \tag{2.3}\\
& \theta(r)=\frac{2 g}{2-\alpha} x^{\beta}+\left(\frac{1}{2}-\nu\right) \pi / 2
\end{align*}
$$

Compare this form of the wavefunction with the quasiclassical solution. The quasiclassical variable phase at $x \ll 1$ is

$$
\int_{x_{1}}^{x}\left[g^{2} x^{-x}-l(l+1) x^{-2}\right]^{1 / 2} \mathrm{~d} x=\left\{2 g x^{\beta}-\pi[l(l+1)]^{1 / 2}\right\}(2-\alpha)^{-1}
$$

As the discrete spectrum is determined by the condition $\theta\left(x_{2}\right)+\pi / 4=(n+1) \pi$ where $x_{2}$ is the larger turning point, we finally get the quantization condition

$$
\begin{equation*}
\int_{r_{1}}^{r_{2}} p(r) \mathrm{d} r=(n+\gamma) \pi, \quad n=0,1,2, \ldots \tag{2.4}
\end{equation*}
$$

$p(r)=\left[2(E-V(r))-\Lambda^{2} r^{-2}\right]^{1 / 2}, \quad \Lambda=[l(l+1)]^{1 / 2}, \quad \gamma=\frac{1}{2}+\frac{l+\frac{1}{2}-\Lambda}{2-\alpha}$.
The centrifugal energy enters the momentum $p(r)$ in its original form (without the Langer substitution), while the constant $\gamma$ depends now on the orbital angular momentum $l$ as well as on the singularity of the potential. The condition (2.4) is a generalization of equation (1.1) applicable for any $l$. On the other hand, at $l \gg 1$

$$
\gamma=\frac{1}{2}+[8(2-\alpha) l]^{-1}+\mathrm{O}\left(l^{-2}\right)
$$

and we obtain the usual quasiclassical condition.
Note that at $n \gg l$ the condition (2.4) may be essentially simplified. In this case $l(l+1) x^{-2} \ll g^{2} v(x)$ in the whole integration region excluding the vicinity of $x_{1}$. With this in mind we omit the centrifugal energy, changing $\gamma$ correspondingly. This procedure results in the following quantization condition:

$$
\begin{equation*}
g Q(\lambda / g)=\left(n+\gamma^{\prime}\right) \pi, \quad \gamma^{\prime}=\frac{2 l+3-\alpha}{2(2-\alpha)} \tag{2.5}
\end{equation*}
$$

where the function $Q(z)$ is defined in (1.2). For $l=0$ the conditions (2.4) and (2.5) are identical. Generalization to the multidimensional case is given in the appendix.

## 3. Bound states with zero energy

The case $E=0$ (appearance of a bound state) is rather interesting. For instance, this problem arises in calculation of the critical nuclear charge, when the electron discrete level drops to the boundary of the lower continuum in the relativistic Coulomb problem (see §5). Let $g_{n l}$ be the value of the coupling constant $g$ at which the bound state with
quantum numbers $n, l$ appears. Defining the function

$$
\begin{equation*}
G(z)=\int_{x_{1}}^{x_{2}}\left[z^{2} v(x)-x^{-2}\right]^{1 / 2} \mathrm{~d} x \tag{3.1}
\end{equation*}
$$

we get from the condition (2.4) an equation to determine $g_{n l}$ :

$$
\begin{equation*}
G(g / \Lambda)=\pi(n+\gamma) / \Lambda, \quad \Lambda=[l(l+1)]^{1 / 2} \tag{3.2}
\end{equation*}
$$

(Here $l>0$; if $l=0$, equation (3.6) is valid.) The function $G(z)$ is real at $z_{0} \leqslant z<\infty$ where

$$
\begin{equation*}
z_{0}=\left(v\left(x_{0}\right)\right)^{-1 / 2} x_{0}^{-1} \tag{3.3}
\end{equation*}
$$

and $x_{0}$ is the root of the equation $x v^{\prime}(x) / v(x)=-2$. When $z \rightarrow z_{0}$ the expansion $G(z)=a_{1}\left(z-z_{0}\right)+a_{2}\left(z-z_{0}\right)^{2}+\ldots$ may be used with coefficients that are expressed in terms of the function $v(x)$ and its derivatives at $x=x_{0}$, eg $a_{1}=\pi\left[z_{0}^{2}\left(3-x^{2} v^{\prime \prime} / 2 v\right)\right]_{x=x_{0}}^{-1 / 2}$.

If $n \ll l$ the root of equation (3.2) is near $z_{0}$ and $g_{n l}$ depends on $l$ approximately linearly:

$$
\begin{equation*}
g_{n l}=c_{1} \Lambda+c_{0}+c_{-1} \Lambda^{-1}+\ldots \tag{3.4}
\end{equation*}
$$

where $c_{1}=z_{0}, c_{0} / c_{1}=(n+\gamma)\left(3-x^{2} v^{\prime \prime} / 2 v\right)_{x=x_{0}}^{1 / 2}$. Thus for the potential

$$
\begin{equation*}
v(x)=\mathrm{e}^{-x} x^{-x}, \quad 0 \leqslant \alpha<2 \tag{3.5}
\end{equation*}
$$

we get $x_{0}=2-\alpha, z_{0}=\left(\mathrm{e} / x_{0}\right)^{x_{0} / 2}, c_{0} / c_{1}=(n+\gamma)\left(x_{0} / 2\right)^{1 / 2}$.
Another limit is $n \gg l$ and $G(z)$ is involved at $z \gg 1$. It may be seen that $G(z)=a z+b+\mathrm{O}(1)$,

$$
a=\int_{0}^{\infty}(v(x))^{1 / 2} \mathrm{~d} x, \quad b=b_{1}+b_{2}, \quad b_{1}=-\pi /(2-\alpha) .
$$

Here $b_{1}$ is determined by the region near $x_{1}$ and $b_{2}$ is from the vicinity of $x_{2} ; b_{2}=0$ if the potential decreases exponentially at large $r$. The result is

$$
\begin{equation*}
g_{n t}=\left(n+\gamma^{\prime}\right) \pi / a, \quad \gamma^{\prime}=\gamma-\frac{b \Lambda}{\pi}=\frac{2 l+3-\alpha}{2(2-\alpha)} \tag{3.6}
\end{equation*}
$$

In this case we also get a linear dependence on $l$; however, the coefficient is different from that in (3.4). The result (3.6) may be deduced from (2.5) by putting $\lambda=0$ and $Q(0)=a$. Note that for the potential (3.5), $a=2^{\beta} \Gamma(\beta), \beta=1-\alpha / 2$.

The conventional quantization condition with the Langer substitution also results in equation (3.2) for $g_{n l}$, where in this case one has to put $\Lambda=l+\frac{1}{2}, \gamma=\frac{1}{2}$. At $l \gg 1$, the difference between the two approaches is negligible:

$$
\Delta g=g_{n l}-g_{n l}^{(\mathrm{L})}=\frac{1}{8 l}\left(\frac{\pi}{a_{1}(2-\alpha)}-z_{0}\right)+\mathrm{O}\left(l^{-2}\right)
$$

(for instance, for the Yukawa potential $\Delta g=-0.0604 l^{-1}$ ).

## 4. Comparison with exact solutions

It is easy to see that for the Coulomb potential, as well as for the oscillator potential, both the quantization conditions (2.4) and (2.5) produce the exact energy spectrum at any $n$ and $l$. Another example of coincidence with the exact solution is the Hulthen
potential at $l=0$. The case is $v(x)=\left(\mathrm{e}^{x}-1\right)^{-1}, Q(z)=\pi\left[\left(1+z^{2}\right)^{1 / 2}-z\right], \gamma=\gamma^{\prime}=1$ and the energy of the $(n+1)$ s level is

$$
\begin{equation*}
\hat{i}=\left[g^{2}-(n+1)^{2}\right] / 2(n+1) \tag{4.1}
\end{equation*}
$$

just as in the exact solution (see eg Flügge 1971).
To test the accuracy of the quasiclassical approach, a wide class of potentials has been considered. The exact spectrum was calculated numerically by means of the variable phase method (Calogero 1967, Marinov and Popov 1973). We present here some of the results.

We start with the problem of appearance of the ground state (ie $n=1, \lambda=0$ ) which seems to be the least appropriate for the quasiclassical approach. For the potentials (3.5) the quantity $\delta=\left(\tilde{g}_{00}-g_{00}\right) / g_{00}$ was calculated, where $\tilde{g}_{00}$ is the exact value of the coupling constant, at which the 1 s level appears, and $g_{00}$ is obtained using the formula (3.6). It is represented in figure 1. If the potential is not too close to the


Figure 1. Relative errors in the quasiclassical calculation for the potential equation (3.5).
singular case $(\alpha \leqslant 1.6)$ the error of formula (3.6) is no more than a few per cent. Analogous results are obtained for the finite-range potential

$$
\begin{equation*}
v(x)=x^{-\alpha} \theta(1-x) \tag{4.2}
\end{equation*}
$$

In this case the exact solution of the Schrödinger equation at $x<1$ (or $r<R$ ) has the form (2.2), while at $x>1, \chi=c_{1} x^{l+1}+c_{2} x^{-l}$. The level appears when the boundary condition $\left(x \chi^{\prime} / \chi\right)_{x=1}=-1$ is fulfilled, so

$$
\begin{equation*}
g_{n l}=\frac{1}{a} \xi_{n+1, v}, \quad a=(1-\alpha / 2)^{-1}, \quad v=\left(l+\frac{1}{2}\right) a-1 \tag{4.3}
\end{equation*}
$$

where $\xi_{n, v}$ is the $n$th positive root of the Bessel function $\mathrm{J}_{v}$. Using the known asymptotics of $\zeta_{n, v}$ (see, eg, Jahnke et al 1960) we get

$$
\begin{equation*}
g_{n l} / g_{n l}=1-\frac{1}{2}(\pi n)^{-2}\left(\nu^{2}-\frac{1}{4}\right)+\ldots \tag{4.4}
\end{equation*}
$$

where $g_{n l}$ is obtained from (3.6) at $\dagger \gamma^{\prime}=(2 v+3) / 4$. Thus one can see that the accuracy of the quasiclassical condition (2.5) is characterized by the parameter $(l / \pi n)^{2}$.
$\dagger$ Note that this value of $y^{\prime}$ is less by $\frac{1}{4}$ than that given in (2.5). This is due to the presence of a sharp edge of the potential well (4.3) at $x=1$.

Consider now the screened Coulomb (Yukawa) potential, $v(x)=\mathrm{e}^{-x} x^{-1}$, which is the most interesting among the potentials (3.5). Results are presented in tables 1 and 2. For the levels $(n+1)$ s from (3.6) one gets $g_{n 0}=(n+1)(\pi / 2)^{1 / 2}$. With increase of $n$ the error falls, while it is of the order $10^{-3}$ at $n=1$. For the levels with $n=0$ and various $l$, two variants of the quasiclassical approximation are presented: ours as well as that obtained from the equation (3.2) with $\Lambda=l+\frac{1}{2}, \gamma=\frac{1}{2}$, corresponding to the Langer approach. The first one is more accurate, and both converge quickly with the exact values when $l$ increases.

Table 1. Coupling constants for the Yukawa potential at which the levels $(n+1) s$ appear ; $g_{n 0}$ are exact values and $g_{n 0}$ are obtained from the quasiclassical equation (3.6).

| $n$ | $\mathfrak{g}_{n 0}$ | $\mathrm{~g}_{n 0}$ |
| :--- | ---: | ---: |
| 0 | 1.296 | 1.253 |
| 1 | 2.539 | 2.507 |
| 2 | 3.787 | 3.760 |
| 3 | 5.037 | 5.013 |
| 4 | 6.288 | 6.267 |
| 5 | 7.540 | 7.520 |
| 6 | 8.791 | 8.773 |
| 7 | 10.044 | 10.027 |
| 8 | 11.297 | 11.280 |

Table 2. Coupling constants at which the levels with $n=0$ and various $l$ appear; $\tilde{g}_{0 l}$ are exact quantities, $g_{01}$ are calculated by means of (3.2), and $g_{0 i}^{(L)}$ result from the conventional formula with the Langer correction.

| $l$ | $\tilde{g}_{01}$ | $g_{01}$ | $g_{01}^{(\mathrm{L})}$ |
| :--- | :---: | :---: | :---: |
| 0 | 1.296 | 1.253 | 1.420 |
| 1 | 3.013 | 3.021 | 3.061 |
| 2 | 4.678 | 4.684 | 4.708 |
| 3 | 6.335 | 6.339 | 6.355 |
| 4 | 7.988 | 7.991 | 8.004 |
| 5 | 9.639 | 9.641 | 9.652 |
| 6 | 11.29 | 11.29 | 11.30 |
| 7 | 12.94 | 12.94 | 12.95 |
| 8 | 14.59 | 14.59 | 14.60 |

The calculations show that when the bound energy increases, the accuracy of the formula (2.4) is also increasing. This was shown for the $s$ levels in some potentials: $v(x)=\mathrm{e}^{-x}, \mathrm{e}^{-x} x^{-1}, \cosh ^{-2} x$. Thus in many cases the quantization condition (2.4), that is asymptotically correct at $n \rightarrow \infty$, predicts the level energies with reasonable accuracy even at low $n$ and $l$.

However, the error of the method is increased when the potential approaches the singular case, $\alpha \rightarrow 2$ (see figure 1). So the question of whether the quasiclassical approach may be applied to singular potentials ( $V(r) \sim r^{-2}$ at $r \rightarrow 0$ ) is to be considered separately.

## 5. Quasiclassical approach to singular potentials

Consider the potential $V(r)=-\beta / 2 r^{2}$. (An effective potential with such a behaviour at $r \rightarrow 0$ arises in the relativistic Coulomb problem for scalar and spinor charged particles (Popov 1970, 1971).) At $\beta>\frac{1}{4}$ the effective orbital angular momentum $l=-\frac{1}{2}+\left[\left(l+\frac{1}{2}\right)^{2}-\beta\right]^{1 / 2}$ becomes complex for the $s$ state. A formal substitution of such $l$ in formulae (2.4) and (2.5) results in complex energies and the method is invalid. As is well known (see, eg, Landau and Lifshitz 1963), at $\beta>\frac{1}{4}$ the 'collapse' occurs. In fact the singular potential cannot be applied to interaction in a real system at small distances, so we introduce a cut-off for $r<r_{0}: V(r)=-\beta f\left(r / r_{0}\right) / 2 r_{0}^{2}$, where $f(1)=1$, $f(0)<\infty$, choosing the point $r_{0}$ so that $\lambda r_{0} \ll 1$. The result is that in the internal region $r<r_{0}$ the solution does not depend on the energy.

In the external region

$$
\begin{equation*}
\chi(r)=r^{1 / 2} K_{\mathrm{iv}}(\lambda r), \quad r>r_{0} . \tag{5.1}
\end{equation*}
$$

We use the condition that the logarithmic derivative is continuous at $r=r_{0}$ and get

$$
\begin{equation*}
x K_{\mathrm{iv}}^{\prime}(x) / K_{\mathrm{iv}}(x)=\xi-\frac{1}{2} \tag{5.2}
\end{equation*}
$$

where

$$
x=\lambda r_{0}, \quad v=\left[\beta-\left(l+\frac{1}{2}\right)^{2}\right]^{1 / 2} ; \quad \xi=\left[r \chi^{-1} \mathrm{~d} \chi / \mathrm{d} r\right]_{r=r_{0}}
$$

is determined by the internal solution. At $\beta>\beta_{\mathrm{cr}}=\left(l+\frac{1}{2}\right)^{2}$ this equation has an infinite number of roots at any $\xi$. One can easily see this from the expansion of $K_{\mathrm{iv}}(x)$ at $x \rightarrow 0$. The discrete spectrum at $\beta \rightarrow \beta_{\mathrm{cr}}$ is given by the formula

$$
\begin{equation*}
E_{n l} \simeq-r_{0}^{-2} c_{l} \exp [-\pi(n+1) / v] \tag{5.3}
\end{equation*}
$$

where $c_{1}$ is a constant depending on $\xi$ and $l$ (see also Morse and Feshbach 1953).
We now obtain the discrete spectrum in the quasiclassical approach. Taking account of the Langer term, $p(r)=\lambda\left[\left(r_{2} / r\right)^{2}-1\right]^{1 / 2}$, where $r_{2}=v / \lambda$ is the turning point. In the region $r_{0}<r<r_{2}$ the quasiclassical wavefunction is

$$
\chi(r)=p^{-1 / 2} \sin \left(\int_{r_{0}}^{r} p(r) \mathrm{d} r+\gamma^{\prime}\right)
$$

The phase shift $\gamma^{\prime}$ is determined from the boundary condition at $r=r_{0}: \nu \cot \gamma^{\prime}=\xi-\frac{1}{2}$. From the Bohr-Sommerfeld quantization condition we have

$$
\gamma^{\prime}+\gamma^{\prime \prime}+\int_{r_{0}}^{r_{2}} p(r) \mathrm{d} r=(n+1) \pi
$$

where $\gamma^{\prime \prime}=\pi / 4$ is a contribution from the turning point $r_{2}$. With the notation $r_{2} / r_{0}=\cosh y$ we obtain

$$
\begin{equation*}
E_{n l}=-\frac{\beta-\beta_{\mathrm{cr}}}{2 r_{0}^{2} \cosh ^{2} y} \tag{5.4}
\end{equation*}
$$

where $y=y_{n l}$ are positive roots of the equation

$$
\begin{equation*}
y-\tanh y=\left[\left(n+\frac{3}{4}\right) \pi-\cot ^{-1} \eta_{l}\right] / v, \quad \eta_{l}=\left(\xi-\frac{1}{2}\right) / v \tag{5.5}
\end{equation*}
$$

The difference between the approximate solution and the exact one obtained from (5.2) diminishes rapidly with the increase in the coupling $\beta$. The reason is that the inequality necessary for application of the quasiclassical approach

$$
\mathrm{d}(p(r))^{-1} / \mathrm{d} r=\left[1-\left(r / r_{2}\right)^{2}\right]^{-3 / 2} / v \ll 1
$$

is better satisfied if $v$ is larger. A consequence of equation (5.4) at $i r_{0} \rightarrow 0$ is the asymptotic formula (5.3). Thus one is able to apply the usual quasiclassical method to the attractive singular potentials if the potential is cut off at small distances.

Using this method we consider the problem of critical nuclear charge. The critical value of the nuclear charge ( $Z_{\text {cr }}>137$ ) is the value of $Z$ at which the ground state atomic level falls up to the boundary of the lower continuum ( $E=-m c^{2}$ ). The quantity $Z_{\text {cr }}$ depends essentially on the nuclear radius $r_{\mathrm{N}}$ and on the charge distribution inside the nucleus. At $Z>Z_{\text {cr }}$ the level dives into the lower continuum and continues as a resonance, $\operatorname{Re} E<-m c^{2}$; the neutral vacuum becomes unstable and an electronpositron pair may be created, the electron occupying the level while the positron is emitted $\dagger$. This problem is now receiving considerable attention in view of a possible test of quantum electrodynamics in the presence of superstrong Coulomb fields (Pieper and Greiner 1969, Popov 1970a, b, 1971, 1973a, Zeldovich and Popov 1971, Mueller et al 1972). The quasiclassical approach for the Coulomb problem with $Z<137$ results exactly in the Sommerfeld fine-structure splitting. Therefore one may hope that even at $Z>137$ the electron energy terms are described accurately by this approach.

By means of the substitution $\chi(r)=r V^{-1 / 2} g(r)$ the Dirac equation at the boundary of the lower continuum is transformed to the Schrödinger form $\chi^{\prime \prime}+k^{2} \chi=0$, where

$$
\begin{align*}
& k^{2}(r)=2 V+V^{2}+\frac{1}{2} V^{\prime \prime} / V-\frac{3}{4}\left(V^{\prime} / V\right)^{2}+r^{-1} V^{\prime} / V \\
& V(r)= \begin{cases}-\zeta / r & \text { at } r>r_{\mathrm{N}} \\
-f\left(r / r_{\mathrm{N}}\right) \zeta / r_{\mathrm{N}} & \text { at } 0<r<r_{\mathrm{N}}\end{cases} \tag{5.6}
\end{align*}
$$

(for the s levels), $\hbar=c=m=1, \zeta=Z \alpha, m$ is the electron mass, $r_{\mathrm{N}}$ is the nuclear radius. Explicit form of the cut-off function $f$ is determined by the charge distribution inside the nucleus. The main contribution to the quantization condition is from the region $r_{\mathrm{N}}<r<r_{1}$ where $r_{1}=\left(\zeta^{2}-1\right) / 2 \zeta$ is the turning point $\left(r_{1} \gg r_{\mathrm{N}}\right)$. In this region

$$
\begin{align*}
& p^{2}=k^{2}-\frac{1}{4} r^{-2}=r^{-2}\left(\zeta^{2}-1\right)\left(1-r / r_{1}\right), \\
& \chi(r)=(r p)^{-1 / 2} \sin \left(\int_{r_{N}}^{r} p \mathrm{~d} r+\gamma^{\prime}\right) \tag{5.7}
\end{align*}
$$

(taking into account the Langer term). Determining the phase $\gamma^{\prime}$ from the boundary condition at the nuclear surface, we have

$$
\gamma^{\prime}+\int_{r_{\mathrm{N}}}^{r_{1}} p \mathrm{~d} r=\left(n+\frac{3}{4}\right) \pi .
$$

$\dagger$ The effect of spontaneous pair creation in a strong electric field is observable in collisions of heavy ions with over-critical total charge ( $Z_{1}+Z_{2}>Z_{\text {cr }}$ ), when the internuclear distance is less than a critical value $R_{\text {cr }}$. For instance, in the case of two U nuclei $R_{\mathrm{cr}} \simeq 50 \mathrm{fm}$, and the corresponding cross sections are rather large (Popov 1973a. Marinov and Popov 1975 and references therein).

The critical nuclear charge $Z_{\mathrm{cr}}=137 \zeta$ as a function of the nuclear radius $r_{\mathrm{N}}$ is obtained from the relation

$$
\begin{equation*}
r_{\mathrm{N}}=\frac{\zeta^{2}-1}{2 \zeta \cosh ^{2} y} \tag{5.8}
\end{equation*}
$$

where $y$ is the root of equation (5.5) where one should put $\eta=\xi\left(\zeta^{2}-1\right)^{-1 / 2}$. As for the constant $\xi$, it is determined by solution of the Dirac equation inside the nucleus and does not depend on the energy at $r_{\mathrm{N}} \ll 1$ (for heavy nuclei $r_{\mathrm{N}} \sim 0.02$ ). To calculate $\xi$ we solve the differential equation for the function $u=\chi / \chi^{\prime}$ :

$$
\begin{equation*}
\frac{\mathrm{d} u}{d \rho}=1+\left[\zeta^{2} f(\rho)+\frac{f^{\prime \prime}}{2 f}+\frac{f^{\prime}}{\rho f}-\frac{3}{4}\left(\frac{f^{\prime}}{f}\right)^{2}\right] u^{2} \tag{5.9}
\end{equation*}
$$

where $\rho=r / r_{\mathrm{N}}, u(0)=0, u(1)=\xi^{-1}$. For example, if the charge is distributed on the nuclear surface, then $f(\rho)=1, \zeta=\zeta \cot \zeta$. It is essential to use equation (5.9) because inside the nucleus the potential is quite different from the Coulomb form and there is no reason to use the quasiclassical method for small $n$. The function $\zeta_{\text {cr }}\left(r_{\mathrm{N}}\right)$, calculated by means of the given formulae for the case of homogeneous charge density (ie $f(\rho)=\left(3-\rho^{2}\right) / 2$ ), is given in figure 2. Results of the exact calculation (Popov 1970) and of the asymptotic estimate (Popov 1972, equation (6)) are also presented.

The asymptotic formula for $\zeta_{\mathrm{cr}}$ is deduced under the assumption that

$$
g=\left(\zeta_{\mathrm{cr}}^{2}-1\right)^{1 / 2} \ll 1,
$$

and the quasiclassical approach is valid at $g \gg 1$. A high accuracy in both calculations, even for the 1 s level, is remarkable. It is seen from figure 2 that these two approximations


Figure 2. Critical charge $\zeta_{\mathrm{cr}}=Z_{\mathrm{cr}} / 137$ for the $1 \mathrm{~s}_{1 / 2}$ electron level as a function of the nuclear radius $r_{\mathrm{N}}$. Curve 1 is the exact solution (Popov 1970), curve 2 is obtained from asymptotical calculation (Popov 1972) and curve 3 is the quasiclassical result.
are found to be valid up to $g \simeq 1$ and the regions of their applicability overlap. The accuracy of the quasiclassical formulae is even better for the excited levels.

It would be of interest to produce a quasiclassical solution of the two-centre problem, obtaining a new estimate for the critical internuclear distance $R_{\text {cr }}$ important for calculation of spontaneous positron production in heavy ion collisions. Note that the asymptotic formula for $R_{\text {cr }}$ was obtained (Popov 1973b) and it was calculated by means of the variational method (Marinov et al 1974).

## Appendix. Multidimensional case

The obtained results may be easily generalized to the case of a spherical symmetric potential in $f$-dimensional space: $V=V(r), r=\left(x_{1}^{2}+\ldots+x_{f}^{2}\right)^{1 / 2}$. The solution of the Schrödinger equation is of the form

$$
\begin{equation*}
\psi_{n i \lambda}=R_{n l}(r) Y_{l \lambda}(\hat{n}), \quad \hat{n}_{i}=x_{i} / r \tag{A.1}
\end{equation*}
$$

where $L^{2} Y_{l \lambda}=l(l+f-2) Y_{l \lambda}, l=0,1, \ldots$, and $\lambda$ is a combination of $f-2$ indices, specifying the $f$-dimensional spherical function. Introducing $\chi(r)=r^{(f-1) / 2} R(r)$ we get the one-dimensional Schrödinger equation $\chi^{\prime \prime}+2(E-U) \chi=0$ where

$$
\begin{equation*}
U(r)=V(r)+L(L+1) / 2 r^{2}, \quad L=l+(f-3) / 2 . \tag{A.2}
\end{equation*}
$$

Thus substituting $l$ by $L$, one may generalize the results to any dimension $f$. In particular, in the quantization condition (2.5) one should use the new value of the constant,

$$
\begin{equation*}
\gamma^{\prime}=\frac{2 l+f-\alpha}{2(2-\alpha)} \tag{A.3}
\end{equation*}
$$

Note that this condition results in exact energy spectra for the Coulomb and oscillator potentials at any $n, l$ and $f$.

Consider now briefly the 'collapse' in $f$ dimensions. For the potential $V(r)=-\beta / 2 r^{2}$ the exact solution has the form (5.1) at $r>r_{0}$, where now $v=\left[\beta-\left(L+\frac{1}{2}\right)^{2}\right]^{1 / 2}$. At $\lambda r_{0} \ll 1$ the quantity $\varsigma$ does not depend on the energy and may be calculated from the equation
$y^{\prime}=1-\left[\beta f(x)-\Lambda(\Lambda+1) x^{-2}\right] y^{2}, \quad \xi=(y(1))^{-1}, \quad y(0)=0, \quad x=r / r_{0}$
where $f(x)$ is the smoothing function. The discrete spectrum arises from the equation (5.2) at $\beta>\beta_{\mathrm{cr}}=(l-1+f / 2)^{2}$. Note that for $l=0$ and $f=2$ the 'collapse' occurs at any positive $\beta\left(\beta_{\mathrm{cr}}=0\right)$. This is due to the form of the effective potential in (A.2). In this case $L=-\frac{1}{2}$ and even for a non-singular potential there is an attraction strong enough, so that the regular and singular solutions differ only by a logarithm: $R_{1} \sim$ constant and $R_{2} \sim \ln r$ at $r \rightarrow 0$. Such a situation is typical for the problems with 'collapse' (Morse and Feshbach 1953).

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