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Bound states in short-range potentials

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Abstract

The bound states in short-range potentials are obtained by solving approximately the integral Schrodinger equation.

We look for bound states of negative energy $E = -\hbar^2 k^2/2m$ of a particle of mass m in a short-range potential well $-|V|$, where k is the wavevector associated with energy E. Schrodinger's equation reads

$$(\Delta - k^2)\psi = -4\pi U\psi \ , \tag{1}$$

where $U = m|V|/2\pi\hbar^2$. Solutions of this equation can be represented by

$$\psi(\mathbf{r}) = \int d\mathbf{r}' \cdot U(\mathbf{r}')\psi(\mathbf{r}')\frac{e^{-k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \ , \tag{2}$$

which is the integral Schrodinger equation. The asymptotic behaviour of this solution reads

$$\psi(\mathbf{r}) = \int d\mathbf{r}' \cdot U(\mathbf{r}')\psi(\mathbf{r}')e^{\mathbf{k}'\mathbf{r}'} \cdot \frac{e^{-k\mathbf{r}}}{r} \ , \tag{3}$$

where $\mathbf{k}' = k\mathbf{r}/r$.

For small values of the potential U equation (2) can be approximated by

$$\psi(\mathbf{r}) = \int d\mathbf{r}' \cdot U(\mathbf{r}')\psi(\mathbf{r}') \cdot \frac{e^{-kb}}{b} \ , \tag{4}$$

where b is the range of the potential. We get immediately the energy level given by

$$k^2 = \frac{1}{b^2}\ln^2\{\frac{1}{b}\int d\mathbf{r}' U(\mathbf{r}')\} \ . \tag{5}$$

We can see that it does not exist unless the potential U exceeds the minimum value given by

$$1 = \frac{1}{b}\int d\mathbf{r}' U_0(\mathbf{r}') \simeq 4\pi b^2 U_0/3 \ , \tag{6}$$

where U_0 is the mean value of the potential. For this threshold value of the potential the energy level is vanishing. For an increase δU the energy level increases (in absolute value) by

$$k^2 \simeq \frac{1}{b^2}(\delta U/U_0)^2 = (4\pi/3)U_0(\delta U/U_0)^2 \ . \tag{7}$$

For deeper potential wells we notice that the main contribution to the eigenvalues equation (2) comes from $\mathbf{r}' \sim \mathbf{r}$. Consequently we write it as

$$\psi(\mathbf{r}) = U \int d\rho \cdot \psi(\mathbf{r}+\rho) \frac{e^{-k\rho}}{\rho} \ , \tag{8}$$

where U is the mean potential and integration is now performed over a range β which depends on $\mathbf{r}$. Equation (8) admits plane waves $e^{i\kappa\mathbf{r}}$ as approximate solutions. Carrying out the integration we get

$$1 = 4\pi U \left\{ \frac{1}{\kappa^2+k^2} - \frac{\cos\kappa\beta + (k/\kappa)\sin\kappa\beta}{\kappa^2+k^2} e^{-k\beta} \right\} \ , \tag{9}$$

for $\kappa\beta \gg 1$. At the same time, equation (2) gives for $\mathbf{r}=0$

$$1 = 4\pi U \left\{ \frac{1}{\kappa^2+k^2} - \frac{\cos\kappa b + (k/\kappa)\sin\kappa b}{\kappa^2+k^2} e^{-kb} \right\} \ . \tag{10}$$

By (9) and (10), for infinitely large potential wells $\beta, b \to \infty$ we get the free, continuos spectrum $k^2 = 4\pi U - \kappa^2$, as expected.

Equation (9) should not depend on $\mathbf{r}$ (through β). For this, its derivative with respect to β must vanish. It gives $\kappa\beta = n\pi$ for all non-vanishing integers $n \neq 0$. The only way to satisfy both equations (9) and (10) is to put $\beta = b$ and quantize κ through $\kappa b = n\pi$. We get the dispersion relation

$$1 = 4\pi U \left\{ \frac{1}{\kappa^2+k^2} - \frac{(-1)^n}{\kappa^2+k^2} e^{-kb} \right\} \ . \tag{11}$$

Making use of (6), it is easy to see that this equation has solutions only for odd integers n. We write therefore the dispersion relations (11) as

$$e^{-kb} + 1 = \frac{\kappa^2+k^2}{4\pi U} \ , \tag{12}$$

for $\kappa b = (2n+1)\pi$, $n = 0, 1, 2, ...$, $4\pi U b^2 \geq 3$ and $\kappa b \gg 1$. We note that κ may run up to a maximum value given by $(\kappa_m b)^2 = 8\pi U b^2$.

For $Ub^2 \gg 1$ the upper bound states are dense; by (12), their energy is given by $kb = 2 - \kappa^2/4\pi U$. With $\kappa = \kappa_m - \delta$ and $\delta b = 2\pi\delta n$ we get the top spectrum $-E = (2\pi\hbar^2/mb^2)^2(\delta n)^2/\left|V\right|$ for a deep potential well.

For deep potential wells ($Ub^2 \gg 1$) the above spectrum is applicale also for the ground state (high values of k), correspondig to the lowest $n = 0$, *i.e.* $\kappa b = \pi$. The ground state energy is easily obtained from (12) in this case as $-E_0 = \left|V\right| - \pi^2\hbar^2/2mb^2$.

Spectrum (12) is also applicable for shallow U, when there is only one bound state. It is given by $kb = 2 - \kappa^2/4\pi U$ for $\kappa b = \pi$. The critical depth is given by $U_0 b^2 = \pi/8$, which differs slightly from (6) ($U_0 b^2 = 3/4\pi$). The level goes like $kb = 2(\delta U/U_0)$, or $k^2 = (32/\pi)U_0(\delta U/U_0)^2$, which again differs from (7) by a numerical factor.

According to the derivation given above the approximate eigenstates are plane waves, with spatial degeneracy. They are more appropriate for s-waves for central potentials, as the l-waves depend more on the details of the potential shape. For deep potential wells the number of energy levels is $\sim (8\pi U b^2)^{1/2}$ (so that the mean distance between energy levels is $\delta E \sim (Ub^2)^{1/2}$) and the number of states is $\sim 4\pi(8\pi U b^2)^{3/2}/3$. They read $(\left|V\right|/\varepsilon)^{1/2}$ and, respectively $\sim (\left|V\right|/\varepsilon)^{3/2}$, where $\varepsilon = \hbar^2/mb^2$ is the localization energy in the potential well.