

Lecture 3 Single-particle QM in 1, 2 and 3D

Consider a single nonrelativistic particle of mass m moving in d dimensions in a conservative, velocity-independent potential $V(\mathbf{r})$. In stationary state it satisfies the TISE*

$$\left(-\frac{\hbar}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad \nabla^2 \equiv \sum_{i=1}^d \partial^2 / \partial x_i^2 \quad (*)$$

The same equation applies to two particles of mass m_1, m_2 moving in a mutual potential $V(\mathbf{r}_1 - \mathbf{r}_2)$ provided that \mathbf{r} is interpreted as the relative coord. $\mathbf{r}_1 - \mathbf{r}_2$ (the COM wave function factors out) and m is replaced by the reduced mass $\mu \equiv (m_1^{-1} + m_2^{-1})^{-1}$. We will consider for simplicity (in 2D and 3D) only the case of a **central** potential, $V(\mathbf{r}) = V(|r|)$. (In 1D, analogous condition is $V(x) = V(-x)$)

3D problems (recap)

A. The bound-state problem

We must solve the TISE (*) subject to the boundary conditions, which crudely speaking imply conditions (a) $\psi(\mathbf{r}) \rightarrow 0$ for $|\mathbf{r}| \rightarrow \infty$ in any direction, (b) $\psi(\mathbf{r})$ cannot behave as negative power of r for $(\mathbf{r}) \rightarrow 0$ **unless** the potential is infinite at the origin (e.g. δ - f 'n or Coulomb). The first condition evidently $\Rightarrow E < 0$.

Standard procedure: separation of variables

$$\psi(\mathbf{r}) = R_\ell(r) Y_{\ell m}(\theta, \varphi)$$

then the radial wave function obeys the differential equation.

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left(r^2 \frac{dR_\ell}{dr} \right) + \left(V(r) + \frac{\hbar^2}{2m} \ell \frac{(\ell+1)}{r^2} \right) R_\ell(r) = ER_\ell(r) \quad (\dagger)$$

If we introduce $\chi_\ell(r) \equiv rR_\ell(r)$, then χ_ℓ satisfies the 1D-like equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \chi_\ell(r) + \left\{ V(r) + \frac{\hbar^2}{2m} \ell \frac{(\ell+1)}{r^2} \right\} \chi_\ell = E\chi_\ell(r)$$

The boundary condition at ∞ is simple ($\chi_\ell(r) \rightarrow 0$); however, the boundary condition at the origin needs some care. If for example $\chi_\ell(r) \rightarrow \text{const.}$ as $r \rightarrow 0$, then $R_\ell(r) \sim 1/r$ and derivative is discontinuous at $r=0$. This is allowed only for $V(0) = \infty$ (i.e. δ -function). Thus, if V is finite at the origin $\chi_\ell(r)$ must tend to zero at least as r . This is actually assumed automatically for the case $\ell \neq 0$ (since the asymptotic form is r^ℓ or $r^{-(\ell+1)}$ and the second must be excluded), but for the s-wave case it must be imposed explicitly. Thus the case of s-wave scattering in a 3D central

* With b.e.'s: (a) single-valued (b) square – integrable (c) gradient continuous except at points where V infinite.

potential is **not** equivalent to a 1D problem with $V(r) \rightarrow V(x)$. In particular, there is no general theorem that for a potential which is everywhere attractive, a bound state must exist; in fact, in specific cases (e.g. 3D square well) it is straightforward to show that the well must be of a certain minimum depth/extent to bind a particle.

B. Scattering (e.g. LL* § 122)

Statement of problem:

incoming wave $\sim \exp ikz$

We are interested in probability of observing scattered particle at ∞ in direction (θ, φ) . Apart from constant factor of k , this is prop to $|\psi|^2(r, \theta, \varphi)$ for $r \rightarrow \infty$. Standard procedure: split wave function into partial-wave components:

$$\psi(\mathbf{r}) = \sum_{\ell m} c_{\ell m} Y_{\ell m}(\theta, \varphi) R_{\ell m}(r)$$

then each partial wave satisfies (\dagger) but now with **positive** $E \equiv \hbar^2 k^2 / 2m$; if we choose z-axis along direction of incidence, then since potential is central, all terms with $m \neq 0$ vanish and we are left with

$$\psi(r) = \sum_i c_i P_\ell(\theta) R_\ell(r) \quad (\ddagger)$$

The functions $R_\ell(r)$ must satisfy the equation (\dagger), which for sufficiently large r (such that $V(r) \rightarrow 0$ are $k^2 r^2 \gg \ell(\ell + 1)$) becomes simply

$$\frac{1}{r^2} \frac{d}{dr} r^2 \frac{dR_\ell}{dr} + k^2 R_\ell(r) = 0$$

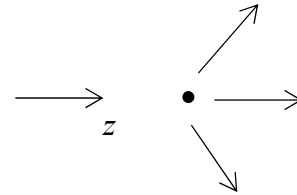
or in terms of $\chi_\ell(r) = rR_\ell(r)$,

$$\frac{d^2 \chi_\ell}{dr^2}(r) + k^2 \chi_\ell(r) = 0$$

The general solution is obviously an arbitrary linear combination of an outgoing wave e^{ikr} and an incoming one e^{-ikr} . It is convenient to write this combination in the form

$$\chi_\ell(r) = \frac{(2\ell + 1)}{k} A_\ell \sin(kr - \ell\pi/2 + \delta_\ell) \quad (A_\ell \text{ complex}) \quad (\S)$$

(note $\delta_\ell \equiv \delta_\ell(k)$!)



* Landau & Lifshitz, Quantum Mechanics, 1965 edition.

where the overall magnitude takes care of the constant c_ℓ in (§). Then the complete form of $\psi(\mathbf{r})$ in the limit $r \rightarrow \infty$ is

$$\psi(\mathbf{r}) = \sum_{L=0}^{\infty} (2L+1) A_L P_L(\cos\theta) \frac{\sin\left(kr - \frac{1}{2}L\pi + \delta_L\right)}{kr}$$

However only part of this corresponds to the scattered wave. If we write

$$\psi(\mathbf{r}) = e^{ikz} + \psi_{sc}(r)$$

then ψ_{sc} must contain only an “outgoing” part (and this must be true for each partial wave component separately). Now we have for $r \rightarrow \infty$

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{\ell} (2\ell+1) i^\ell P_\ell(\cos\theta) \sin\left(kr - \frac{1}{2}\ell\pi\right)$$

so this condition gives

$$A_\ell = i^\ell e^{i\delta_L}$$

and the coefficient of the ℓ -th outgoing partial wave is

$$f_\ell \equiv e^{2i\delta_\ell} - 1$$

Hence, finally, the complete outgoing wave has the form for $r \rightarrow \infty$

$$\psi_{sc}(\mathbf{r}) = f(\theta) \frac{e^{ikr}}{r}, \quad f(\theta) = \sum_{L=0}^{\infty} (2L+1) \left(\frac{e^{2i\delta_L} - 1}{2ik} \right) P_L(\theta)$$

and the scattered intensity is $|f(\theta)|^2$.

The total scattering cross-section σ is $\int |f(\theta)|^2 d\Omega$, thus $\left(\int P_\ell(\theta) P_{\ell'}(\theta) d\Omega = \frac{4\pi}{2L+1} \delta_{\ell\ell'} \right)$

$$\sigma = \frac{1}{4} \sum_{\ell=0}^{\infty} (2\ell+1) \frac{|e^{2i\delta_\ell} - 1|^2}{k^2} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell(k)$$

Hence the phase shifts $\delta_\ell \equiv \delta_\ell(k)$ give complete information on the scattering. They are obtained by solving the complete equation, valid for all r ,

$$\frac{-\hbar^2}{2m} \frac{d^2}{dr^2} \chi_\ell(r) + \left\{ V(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r} \right\} \chi_\ell = E \chi_\ell(r)$$

subject to the boundary condition at $r = 0$, and matching to the asymptotic form (§) in the limit $r \rightarrow \infty$

A particularly interesting case arises when $kr_0 \ll 1$ where r_0 is the range of the potential $V(r)$. In this case, since $R_\ell \sim (kr)^\ell$ for $kr \ll 1$, the partial waves with $\ell \neq 0$ never “feel” the potential and for them $\delta_\ell \approx 0$. Thus the only relevant partial wave is the s-wave component. In this case it is easier to proceed as follows: Assume for the moment that the scattering is not too “strong” (see below), and consider the limit $k \rightarrow 0$. There in the region $kr \ll 1$ but $r \gg r_0$, the TISE reduces simply to the Laplace equation $\nabla^2 \psi = 0$, and the most general form of the s-wave (spherically symmetric) solution is apart from normalization

$$\psi = \psi(r) = 1 - a_s/r$$

where a_s is defined as the zero-energy s-wave scattering length. It can be positive or negative. Under most circumstances, the value of $|a_s|$ is comparable to the range r_0 of the potential; however, close to the onset of a bound state it can be $\gg r_0$. In fact, as we approach the ground state from above, $a_s \rightarrow \infty$, and as we approach it from below (i.e. as the bound state rises into the continuum) $a_s \rightarrow +\infty$.

From the point of view of the scattering problem, a given value of a_s is equivalent to the effect of a δ -function pseudopotential

$$\boxed{V_{ps}(r) = \frac{2\pi\hbar^2}{m} a_s \delta(r)} \equiv g\delta(r)$$

The simplest way to see this is to note that the general form of the s-wave solution of the zero-energy TISE

$$\frac{-\hbar^2}{2m} \nabla^2 \psi + \frac{2\pi\hbar^2}{m} a_s \delta(r) \psi(r) = 0$$

is precisely (constant $-a_s/r$), and we must fix the constant to give the right result for $r \gg a_s$, so we recover the above form $\psi(r) = 1 - a_s/r$. It is also straightforward to show that the energy shift of a (low-energy) particle contained in a spherical box with a scattering potential near the origin such that the zero- E scattering length is a_s is just $(2\pi\hbar^2 a_s/m) |\psi(0)|^2$. (where $\psi(0)$ is calculated in the absence of the potential.) Alternatively, we can say that in 3D, for a δ -function potential of strength g , the scattering length $a_s \propto g$.

Finally, we note that from the above definitions $a_s \equiv f_0$ and hence, by equation (\ddagger)

$$\delta_0(k) = ka_s \quad (k \rightarrow 0)$$

1 dimension

A. Bound states

In 1D the TISE is simply

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{dx^2} + v(x) \right] \psi(x) = E\psi(x)$$

We will not necessarily assume that V is parity-invariant (i.e. $V(x) = V(-x)$). The boundary conditions are that $\psi(x)$ is single-valued, square-integrable and has a continuous first derivative except possibly at points at where $V(x)$ is infinite. The square integrability condition clearly implies that $\psi(x) \rightarrow 0$ as $|x| \rightarrow \infty$, which in turn implies $E < 0$.

We will show that for any form of $V(x)$ s.t. $V(x) \leq 0$ everywhere, at least one bound state always exists.

Proof: Consider some range R of x , say $-a < x < a$, such that it is not true that $V(x) = 0$ everywhere in R . Construct the variational wave function

$$\psi(x) = A, \quad x \in R$$

$$\psi(x) = \exp(-|x - a \cdot \text{sgn} x| / 2A), \quad x \notin R$$

The normalization condition then $\Rightarrow A = [2(a + \lambda)]^{-1/2}$. The expectation value of the energy of the above state is composed of potential and kinetic terms: since the potential contribution from $x \notin R$ is negative (or zero) we have the upper limit

$$\langle E \rangle \leq A^2 \left(-V_0 + \frac{\hbar^2}{8m\lambda^2} \right) = \left(-|V_0| + \frac{\hbar^2}{8m\lambda^2} \right) / 2(a + \lambda) \quad (*)$$

where

$$|V_0| \equiv \left| \int_{-a}^a V(x) dx \right|$$

It is clear that however small $|V_0|$, we can always find a value of λ large enough that the RHS of (*) is < 0 . Thus at least one bound state always exists QED.

To see why an analogous result doesn't follow in 3D, imagine imposing the condition that $\psi(x)$ vanish at some point, say $x=0$. Then the minimum bending energy required **within** the range $-a < x < a$ is of order $A^2 \cdot \hbar^2/2ma$; effectively this adds a constant a^{-1} to the λ^{-1} , in the numerator of (*), and it can no longer necessarily be made negative.

[Problem on odd-parity state.]

Scattering

We consider scattering of an incident wave from $-\infty e^{ikx}$, by a potential $V(x)$ (not necessarily symmetric) which occupies a finite region of the x -axis around $x=0$.

Since in the potential-free region the solution of the TISE must satisfy

$d^2\psi/dx^2 + k^2\psi = 0$ ($k \equiv (2m/\hbar^2)^{1/2}$), the most general solution in that region is (since there is no wave incident from $x=+\infty$)

$$\begin{aligned}\psi(x) &= e^{ikx} + r e^{-ikx}, & x < 0 \\ &= t e^{ikx} & x > 0\end{aligned}$$

where r and t are the (complex) reflection + transmission coefficients. From the conservation of current it is clear that

$$|r|^2 + |t|^2 = 1$$

We can also consider the case of a wave incident from $+\infty$ in which case the reflection and transmission coefficients are defined to be r' and t' respectively. In fact, we can write down a “scattering matrix”

$$S = \begin{matrix} & + & - \\ \begin{matrix} + \\ - \end{matrix} & \begin{pmatrix} r & t \\ t' & r' \end{pmatrix} \end{matrix}$$

Since this matrix must be unitary (so as to preserve the normalization of an incoming arbitrary combination of e^{ikx} and e^{-ikx}), we have $SS^\dagger = 1$, i.e.

$$|t|^2 + |r|^2 = |t'|^2 + |r'|^2 = 1 \quad (\text{as before})$$

$$t/r = -(t'/r')^* \quad \Rightarrow \quad |t| = |t'|, \quad |r| = |r'|$$

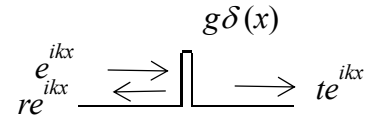
Note that the phase of t is physically meaningful (e.g. we could interfere the transmitted beam with one which has avoided the scatterer) but the phase of r is essentially a question of the choice of origin, so without loss of generality we can take r real. For a **symmetric** potential ($V(x) = V(-x)$) we can take $r = -r'^*$ and $t = t'^*$, so the problem is completely specified by the single complex number t . For the more general case, however, it may differ from t' in phase (though not in amplitude) [Prob.] Evidently we can define a “scattering length” a by $t = |t| e^{ike}$.

It is interesting to study the special case of a δ -function potential, $V(x) = g\delta(x)$. Recall that in 3D, for a potential $g\delta(r)$, we find a low-energy s-wave scattering length $a_s = g/(2\pi\hbar^2/m)$. Now in 1D the dimensions of g are different (EL as opposed to EL^3) so it is obvious on these grounds alone that the above relation does not hold. So what **is** the relation between g and a ?

We match the wave function itself at

$x = 0$ giving

$$r = t - 1$$



Integration of the TISE across the origin gives

$$\Delta \left(\frac{\partial \psi}{\partial x} \right) \left(\equiv \frac{\partial \psi}{\partial x}(x=0+) - \frac{\partial \psi}{\partial x}(x=0-) \right) = + \frac{2mg}{\hbar^2} \psi(0)$$

but

$$\Delta(\partial \psi / \partial x) = ik(t - (1-r)) = 2ik(t-1) \quad , \quad \psi(0) = t$$

so:

$$ik(t-1) = (mg / \hbar^2)t$$

$$t = \frac{1}{1 - mg / ik\hbar^2} \quad (\text{note } < |t| < 1 \text{ and } \rightarrow 0 \text{ as } k \rightarrow 0)$$

If we define “even” and “odd” scattering amplitudes by

$$\psi_x \equiv \psi - e^{ikz} \equiv f_{\text{even}}(e^{ikx} + e^{-ikx}) + f_{\text{odd}}(e^{ikx} - e^{-ikx})$$

then from $1 + r = t$ we have $f_{\text{odd}} = 0$,

$$f_{\text{even}} \equiv t - 1 = \frac{1}{1 - \frac{ik\hbar^2}{mg}} = \frac{1}{1 + ik a_{1D}}$$

where the “1D scattering length” a_{1D} is defined by

$$a_{1D} \equiv \frac{-\hbar^2}{mg}$$

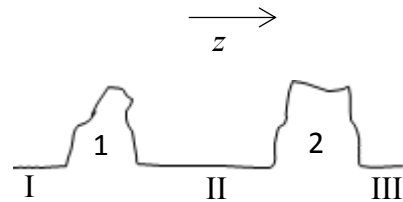
so a_{1D} is inversely proportional to g and opposite in sign.

(note that in the limit $k \rightarrow 0$ this agrees with our previous definition $t = |t| e^{ika}$)

Two barriers in series

It is worth discussing this problem here because it will be needed for the discussion of localization in lecture 4.

Suppose that there are two distinct barriers separated by a region of zero potential (II); note that the length of II does not have to be large compared to the width of the barriers, all we need is to be able to define an “asymptotic” behavior.



Suppose a particle is incident from $z = -\infty$ with momentum $\hbar k$, i.e. the incoming wave is $\exp(ikz)$. Then in the various $V = 0$ regions we have

$$\text{I: } \psi(z) = \exp ikz + A \exp -ikz$$

$$\text{II: } \psi(z) = B \exp ikz + C \exp -ikz$$

$$\text{III: } \psi(z) = D \exp ikz$$

so that the transmission coefficient is $|D|^2$ and the reflection coefficient is $|A|^2$. How are these quantities related to the reflection and transmission coefficients of the two barriers individually?

To see this, we note that

$$\left. \begin{array}{l} A = r_1 + t_1' c \\ B = t_1 + r_1' c \\ C = r_2 B \\ D = t_2 B \end{array} \right\} \Rightarrow B = \frac{t_1}{1 - r_1' r_2}$$

$$\left. \begin{array}{l} C = r_2 B \\ D = t_2 B \end{array} \right\} \Rightarrow D = \frac{t_1 t_2}{1 - r_1' r_2}$$

The total transmission coefficient $T_{12} \equiv |D|^2$ is therefore given (since $|t_1|^2 = T_1$, $|r_1'|^2 = R$, etc.) by the expression

$$T_{12} = \frac{T_1 T_2}{|1 - r_1' r_2|^2}$$

In evaluating the quantity $r_1' r_2$, we must have in mind that it implicitly includes a phase shift φ , where $\varphi = ka$, a being the difference between the “origins” chosen for behaviors 1 and 2. (Recall that the phase of r is a matter of convention which depends on this origin). Thus, defining $\theta \equiv 2\varphi + \arg(r_1' r_2)$ (where r_1' no longer includes the phase shift) we find $(1 - r_1' r_2) = 1 - \sqrt{R_1 R_2} e^{i\theta}$ and hence

$$T_{12} = \frac{T_1 T_2}{1 + R_1 R_2 - 2\sqrt{R_1 R_2} \cos \theta}$$

which is the required result. Using the relations $t_1 / r_1 = -(t_1' / r_1)^*$ etc., it may be verified with some labor that $R_{12} = 1 - T_{12}$

Note that in the limit of large reflectance, T_{12} can actually be larger than $T_1 T_2$ (cf. the situation in a Fabry-Perot etalon.)

2 dimensions

Note that the problem of scattering (or bound states) in 2D is relevant not only to “truly” 2D systems, but to 3D ones with cylindrical symmetry (e.g. a charged particle in the field of a long straight charged wire). The 2D problem is considerably trickier than the 1 or 3D ones, in part because there is no limit which it can be reduced to an essentially 1D one.

The Schrödinger equation in polar coordinates r, φ can be separated by writing

$$\psi(r) = \exp(in\varphi) \cdot R(r) \quad n = -, \pm 1, \pm 2 \dots \text{ (but see below)}$$

The radial wave function now obeys

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d}{dr} r \frac{dR_n}{dr}(r) + \frac{n^2 \hbar^2}{2mr^2} R_n + V(r)R_n(r) = ER_n(r)$$

Unlike the case of 3D there is now no transformation which reduces this to a simple 1D TISE, even for $n = 0$. The most obvious substitution is $\chi_n(r) = r^{1/2} R_n(r)$, but this gives

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \chi_n + \left(n^2 - \frac{1}{4}\right) \frac{\hbar^2}{2mr^2} \chi_n + V(r)\chi_n(r) = E\chi_n$$

and no simple transformation will get rid of the $1/4$.

However, it is amusing that we can cancel this term by application of an appropriate Aharonov-Bohm flux. Suppose the system is pierced by a thin tube containing a flux Φ such that no field leaks out into the region where the particle is. We describe this by a magnetic vector potential $A(r) = \hat{\varphi} \times \Phi / 2\pi r$, and the effect is to replace $-i\partial / \partial\varphi$, in the angular part of the KE, by $-i\partial / \partial\varphi - (e/\hbar) A_\varphi = i\partial / \partial\varphi - (e/h)\Phi$. As before, to ensure single-valuedness the angular wave function must be of the form $e^{im\varphi}$, but now the associated KE is not $n^2 \hbar^2 / 2mr^2$ but rather $(\hbar^2 / 2mr^2) (n - \Phi/h)^2$, where Φ is the single particle flux quantum h/e . We see that if Φ is **exactly half a flux quantum** and $n = 0$, then the flux term exactly cancels the $1/4$ in (*) and we indeed get the simple “1D” form of the radial wave equation, just as in the 3D case.

The theory of scattering in 2D can be analyzed similarly to the 3D case*. In this case the free-space solutions of the radial SE (*) are the Bessel and Neumann functions† $J_n(kr)$, $N_n(kr)$, and the appropriate circular expansion of an incoming wave is

$$\exp(ikz) = \sum_{n=-\infty}^{\infty} i^n \exp(in\varphi) \cdot J_n(kr)$$

* S. Adhikari, Am. J. Physics **S4**, 362 (1985); M. Randeria et al. PRB **4**, 327 (1990)

† Abramowitz Stegun, Ch 9. The function $N_n(*)$ is often identical $Y_n(x)$ and called a Bessel function of the same kind.

There is no great point in going through the details, but note that the S -wave phase shift $\delta_0(k)$ for $k \rightarrow 0$ (which in 3D is ka_s , and in 1D ka_{1D} , cf. above) in 2D **diverges logarithmically**:

$$\delta_0^{(2D)}(k) \dots \cong \frac{1}{2\pi} \ln(k\tilde{a})$$

where \tilde{a} is a characteristic length of the potential, which however should probably not be thought of as a scattering length.

Bound States: We have seen that a purely attractive potential (or more generally one whose space integral is < 0) will always sustain at least one bound state in 1D, but not necessarily in 3D. What is the result in the 2D case? Because of the rather awkward properties of the Bessel and Neumann functions, it is actually easier to look at the problem in k -space rather than in r -space. The k -space form of the TISE is (in any dimension)

$$(\varepsilon_k - E)\psi_k = -\sum_k V_{kk'}\psi_{k'} \quad (V_{kk'} \equiv V_{k-k'})$$

Let's consider a very extended state, such that all k' are $\ll r_0^{-1}$, the inverse range of the potential. Then we should be able to replace $V_{kk'}$ by the constant $V_0 \equiv \int V(r)dr$ and the TISE reduces to

$$1 = -V_0 \sum_k (\varepsilon_k - E)^{-1}$$

It is clear that, whatever d , this equation has no bound state ($E = 0$) solution if $V_0 > 0$. If $V_0 < 0$, then everything depends on the density of states as k (or E) $\rightarrow 0$. The sum over k becomes in d dimensions $c_d \int d \in \in^{(d-2)/2}$, where c_d is a constant; in particular $c_2 = (m / 2\pi\hbar)$. Thus the TISE reads

$$1 = |V_0| c_d \int d \in \frac{\in^{(d-2)/2}}{\in - E}$$

(for \in_c , see below)

It is clear that this equation always has an $E < 0$ solution for $d = 1$; for $d = 3$ it may or may not depending on the high energy cutoff \in_c (which must be determined e.g. by the departure of $V_{k-k'}$ from constant value V_0 and so is typically $\sim \hbar^2 / mr_0^2$). For $d = 2$ a solution always exists, but the binding energy is exponentially small for

$$V_0 \rightarrow 0:$$

$$E \approx \in_c \exp[-1 / (mV_0 / 2\pi\hbar^2)]$$

(cf. the solution of the Cooper problem is superconductivity theory, which is formally identical to a simple 2D Schrödinger problem since the relevant density of states is similarly a constant.)