

Lecture 8

Single-particle QM in 1, 2 and 3D

Consider a single nonrelativistic particle of mass m moving in a d -dimensional ^{in a} conservative, velocity-independent ^{pot.} $V(\underline{r})$. We describe the stationary state & satisfies the TISE*

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

The same eqn. applies to two particles ~~mass~~ of masses m_1, m_2 moving in a mutual pot. $V(\underline{r}_1 - \underline{r}_2)$ provided that \underline{r} is interpreted as the relative coord. $\underline{r}_1 - \underline{r}_2$ (the COM wf 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 or 3D) only the case of a central pot., $V(\underline{r}) = V(|r|)$ (in 1D, analogous condition is $V(x) = V(-x)$)

3D problem (recap)

A. The bound-state problem

We must solve the TISE (*) subject to the ^{b.} ~~boundary~~ ^{conditions} $\psi(\underline{r}) \rightarrow 0$ for $|\underline{r}| \rightarrow \infty$ in any direction, (b) $\psi(\underline{r})$ cannot blow up anywhere ^{of \underline{r}} for $\underline{r} \rightarrow \infty$ unless the potential is infinite at the origin (eg δ -fn or Coulomb). The first Sturm-Liouville condition evidently $\Rightarrow E < 0$.

Standard procedure: separation of variables

$$\psi(\underline{r}) = R_l(r) Y_{lm}(\theta, \varphi)$$

then the radial wf obeys the diff. eqn.

$$-\frac{\hbar^2}{2m r^2} \frac{d}{dr} \left(r^2 \frac{dR_l}{dr} \right) + \left(V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) R_l(r) = E R_l(r) \quad (*)$$

If we introduce $\chi_l(r) \equiv r R_l(r)$, then χ_l satisfies the 1D-like eqn.

* with b.c.'s: (a) single-valued (b) square-integrable (c) gradient continuous except at points where $V \rightarrow \infty$.

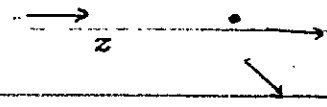
$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \chi_\ell(r) + \left\{ V(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right\} \chi_\ell(r) = E \chi_\ell(r)$$

The boundary condition at ∞ is simple ($\chi_\ell(r) \rightarrow 0$); however, the b.c. 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 deriv. is discontinuous at $r=0$. This is allowed only for $V(0) = \infty$ (eg. δ -function) or δ -like potential. 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 $\ell=0$ case it must be imposed explicitly. This in case of $\ell=0$ scattering in a 3D central potential is not equivalent to a 1D problem with $V(r) \rightarrow V(r)$. In particular, there is no general theorem that for a pot. which is everywhere attractive a bound state must exist; in fact, in specific cases (eg. 3D square well) it is straightforward to show that there will not be if a certain minimum depth / extent is not reached.

B. Scattering (eg. L.C. § 122)

Statement of problem:

incoming wave $\sim \exp(ikz)$



We are interested in prob. of observing scattered particle at ∞ in dir. (θ, ϕ) and geom. prob. $1/r^2$

After time conv. factor of k , this is prob. $\propto |\psi(r)|^2$ at ∞ (r, θ, ϕ) for $r \rightarrow \infty$.

Standard procedure: split w/f into partial-wave comp's:

$$\psi(r) = \sum_{\ell m} c_{\ell m} Y_{\ell m}(\theta, \phi) R_{\ell m}(r) \quad \equiv \hbar^2 k^2 / 2m$$

then each partial wave satisfies (*) but now with positive E . If we choose z -axis along dir. of incidence, then since pot. is central all terms with $m \neq 0$ vanish out or on left with

$$\psi(r) = \sum_{\ell} c_{\ell} P_{\ell}(\cos \theta) R_{\ell}(r) \quad (**)$$

Split of into "incoming" and "outgoing" waves:

The function $R_l(r)$ must satisfy the eqn (†), which for sufficiently large r (such that $V(r) \rightarrow 0$ and $k^2 r^2 \gg l(l+1)$) becomes simply

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} r^2 \frac{dR_l}{dr} + k^2 R_l(r) = 0$$

or in terms of $\chi_l(r) \equiv r R_l(r)$,

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

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

$$\chi_l(r) = \frac{(2l+1)A_l}{k} \sin(kr - \frac{1}{2}l\pi + \delta_l) \quad (A_l \text{ complex}) \quad (3)$$

(note $\delta_l \equiv \delta_l(k)$!)

When the overall sign A_l is chosen of the constant C_l in (†). Then the complete form of $\psi(r)$ in the limit $r \rightarrow \infty$ is

$$\psi(r) = \sum_{l=0}^{\infty} (2l+1) A_l P_l(\cos \theta) \sin(kr - \frac{1}{2}l\pi + \delta_l)$$

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

$$\psi(r) = e^{ikz} + \psi_s(r)$$

then ψ_s must contain only an "outgoing" part. Now we have for $r \rightarrow \infty$

$$e^{ikz} = e^{ikr \cos \theta} \rightarrow \sum_l (2l+1) i^l P_l(\cos \theta) \sin(kr - \frac{1}{2}l\pi)$$

so this condition gives

$$A_l = i^l e^{i\delta_l} \quad (\text{scat})$$

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

$$f_l \equiv e^{2i\delta_l} - 1$$

Hence, finally, the ^{complex} outgoing wave has the form for $r \rightarrow \infty$

$$f \psi_{sc}(r) = f(\theta) \frac{e^{ikr}}{ikr} \quad f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) (e^{2i\delta_l} - 1) P_l(\theta)$$

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

The total scattering cross-section is $\int |\psi(\theta)|^2 d\Omega$, thus $\int P_l(\theta) P_l(\theta) d\Omega = \frac{4\pi}{2l+1} \delta_{l,0}$

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

$$\equiv \delta_l(k)$$

Here the phase shifts δ_l give complete info on the scattering. They are obtained

by solving the complete equation, valid for all r .

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

and subject to the b.c. at $r=0$, and matching to the asymptotic form (3) in the

limit $r \rightarrow \infty$

A particularly interesting case arises when $kr_0 \ll 1$ when r_0 is the range of the pot. $V(r)$. In this case, since $\chi_l \sim R_l \sim (kr)^l$ for $kr \ll 1$,

the partial waves with $l \neq 0$ never "feel" the potential and for them $\delta_l \approx 0$.

Thus the only relevant p.w. is the s-wave comp. In this case it is easier

to proceed as follows: we simply solve the A.S. for the minimum that the

scattering is due to "strong" (in this case), and consider the limit $kr_0 \ll 1$, or

$kr_0 \ll 1$ but $r \gg r_0$. Then in the region $kr \ll 1$ but $r \gg r_0$, the most general form of the TISE reduces simply to the Laplace eqn $\nabla^2 \psi = 0$, and the s-wave

(spherically symmetric) solution is, apart from normalization:

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

it can be $l=0$ or $-n$

where a_s is def. as the zero-energy s-wave scattering length. 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 BS from above, $a_s \rightarrow -\infty$, and as we approach it

from below (i.e. as the BS merges into the continuum) $a_s \rightarrow +\infty$.

From the point of view of the scattering process, a given value of a_s

is equivalent to the effect of a δ -function potential

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

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

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

is precisely $\sim a_s/r$, and if $a_s > 0$ we must fix the constant to give the right result for $r \gg a_s$, so in essence the above form $\psi(r) = 1 - a_s/r$ (low-energy) straightforward to show that the energy shift of a particle confined in a 1D potential box with a δ -well at the origin is the zero-energy s -wave length a_s is just $(2\pi\hbar^2 a_s/m) |\psi(0)|^2$ (where $\psi(0)$ is calculated in the absence of the δ -well). Alternatively, we can say that in 3D, for a δ -function potential of strength g , the s -wave length is $a_s = a_g$.

Finally, we note that from the above definition $a_s \equiv f_0$ and hence, by eqn. (†)

$$\delta_0(k) = \hbar a_s$$

($k \rightarrow 0$)

1 dimension

A. Bound states

In 1D the TISE is simply

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

We will not necessarily assume that V is parity-invariant (i.e. $V(x) = V(-x)$). The b.c.'s are that $\psi(x)$ is finite single-valued, square-integrable and has a continuous first derivative except possibly at points 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 $-a < x < a$, where $V(x) \leq 0$.

It is not true that $V(x) = 0$ everywhere in R . Construct the variational w.f.

$$\psi(x) = \frac{A}{\cos \lambda x}, \quad x \in R$$

$$\psi(x) = A \exp(-|x|/\lambda), \quad x \notin R$$

The normalized condition $\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \Rightarrow A = [2(a+\lambda)]^{-1/2}$ (exp. value of λ)
The energy of the

above state is composed of pot. & kinetic terms: since the pot. energy from

$x \notin R$ is $\langle E \rangle$ negative (or zero) we have the upper limit

$$\langle E \rangle \leq A^2 (-V_0 + \frac{1}{2} \lambda^2) = \frac{1}{2} (-V_0 + \lambda^2) / (a+\lambda)$$

where

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

$$\lambda^{-1} \left(\frac{h^2}{2m} \right)$$

It is clear that however small $|V_0|$, we can always find a value of λ small enough that the RHS of (*) is < 0 . Thus at least one b.s. always exists, Q.E.D.

To see why an analysis must describe states in 3D, imagine imposing the condition that $\psi(x)$ vanish at some point, say $x=0$. Then the minimum binding energy required within the range $-a < x < a$ is of order $A^2 \cdot h^2 / 2ma$ effectively this adds a constant $\propto a^{-1}$ to the λ^{-1} , ~~subtraction~~ in the numerator of (*), and it can no longer need to be made $-ve$.

[Prob. in odd-parity states]

Scattering

We consider scattering of an incident wave $\rightarrow e^{ikx}$ 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 $d^2\psi/dx^2 + k^2\psi = 0$ ($k \equiv (2mE/\hbar^2)^{1/2}$), the most general solution is (since there is no wave incident from $x=+\infty$)

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

where r and t are the (complex) reflection & transmission coefficients. For

The conservation of current is clear now

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

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"

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

Since this matrix must be unitary (so as to preserve the norm of ψ on a domain arbitrary constⁿ of e^{ikx} and e^{-ikx}), we have $SS^\dagger = 1$, i.e.

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

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

Note that the phase of t is physically meaningful (eg 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 and $r' = -r^*$. 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 no. t . For the more general case, however, t may differ from t' in phase (though not in amplitude) [Prob.] Evidently we can define a

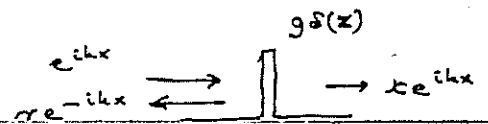
It is interesting to study the special case of a δ -function potential,

$V = g\delta(x)$. Recall that in 3D, for a potential $g\delta(r)$, we had a low-energy s -wave scattering length $a_s = 2\pi^2 g / (2\pi\hbar^2/m)$. Now in 1D ~~we have~~

~~we can define a scattering length~~ the dimension of g is different (EL is opposite to EL²) so it is obvious on dimensional grounds alone that the atom nucleus does not hold. So what is the relation between g and a ?

"scattering length" a by $t = |t|e^{-ika}$.

We match the wave function itself at



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

$$\Delta \left(\frac{\partial \psi}{\partial x} \right) = ik(t - (1-r)) = 2ik(t-1), \quad \psi(0) = t$$

so substituting in above

so:

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

\Rightarrow

$$t = \frac{1}{1 - mg/ik\hbar^2}$$

(note $|t| < 1$!)

and $\rightarrow 0$ as $k \rightarrow 0$.

If we define "even" and "odd" scattering amplitudes by

then from $f_{\text{odd}} + f_{\text{even}} = t$, $f_{\text{odd}} = 0$ and $f_{\text{even}} = t-1$

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

then from $f_{\text{odd}} = 0$ we have $f_{\text{even}} = 0$.

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

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

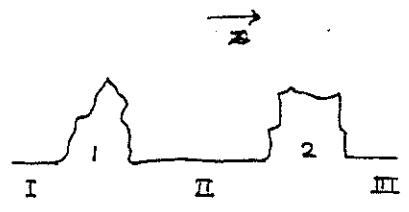
$$a_{1D} \equiv -\frac{\hbar^2}{mg}$$

so a_{1D} is inversely proportional to

and opposite in sign.

Two barriers in series

It is worth discussing this problem here. It will be needed for the discussion of localizⁿ in l. 6. Suppose that there is no definite



barriers separated by a region of zero potential (II); we treat the layers of II des. we have to be large c'd the width of the barriers, all we need is to define an "asymptotic" behavior

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

$$\begin{aligned} \text{I: } \psi(z) &= \exp(ikz) + A \exp(-ikz) \\ \text{II: } \psi(z) &= B \exp(ikz) + C \exp(-ikz) \\ \text{III: } \psi(z) &= D \exp(ikz) \end{aligned}$$

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

To see this, we note that

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

The total transmission coefficient T_{12} is $|D|^2$ is therefore given (since $|t_1|^2 = T_1, |r_1'|^2 = R_1$, 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 bear in mind that it includes phase 2ϕ , where $\phi = ka$, a being the distance between the "origins" chosen for barriers 1 and 2. (Recall that the phase of r is a multiple

convention which depends on his origin). Thus, defining $\theta \equiv \arg 2\varphi + \arg(\dots)$

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 expected result. Using the relations $\arg \epsilon_1/r_1 = -(\epsilon_1/r_1)^*$ etc.

(1.4), it may be verified with some labor that $R_{12} = 1 - T_{12}$, as of course it must be.

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

2 dimensions

(or BS)

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

The Schrödinger eqn. in polar coords r, ϕ can be separated by writing

$$\psi(r) = \exp i \frac{n}{\hbar} \phi R_n(r) \quad n = 0, \pm 1, \pm 2 \dots \text{ (but not } \frac{1}{2} \text{)}$$

The radial wave function now obeys

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

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

$$-\frac{\hbar^2}{2m} \frac{d^2 \chi_n}{dr^2} + \left(\frac{n^2 \hbar^2}{2mr^2} + \frac{\hbar^2}{8mr^2} \right) \chi_n = E \chi_n \quad (-VR_n)$$

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

However, it is amusing that we can cancel this term by application of an appropriate AB flux. Suppose the system is pierced by a thin tube containing a flux Φ , i.e. no field leaks out into the region where the particle is. We describe this by a magnetic vector potential $\vec{A}(r) = \hat{\phi} \times \Phi / 2\pi r$, and

the effect is to replace $i\partial/\partial\phi$ in the angular part of the KE, by

$$-i\partial/\partial\phi - (e/\hbar) A_\phi = i\partial/\partial\phi - (e/\hbar) \Phi$$

As before, the angular wave functions must be of the form $e^{im\phi}$, but now the associated KE is not $n^2 \hbar^2 / 2mr^2$ but rather $(\hbar^2 / 2mr^2) (n - \Phi/\Phi_0)^2$, where

Φ_0 is the (s-b) flux quantum h/e . We see that if Φ is exactly half a flux quantum, then the flux term exactly cancels the $1/4$ in (*) and we can indeed get the simple "1D" form of the radial wave equation $\ddot{\chi}$, just as in the 3D case

The theory of scattering in 2D can be developed 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

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

There is no great point in going through the details, but note that the s-wave phase shift $\delta_0(k)$, (which, in 3D is $k a_0$, and in 1D $-ka_0$, cf. above) in 2D diverges logarithmically:

$$\delta_0^{(2D)}(k) \approx \frac{1}{2\pi} \ln(k_0 \bar{a})$$

where \bar{a} is a characteristic length, which here would probably be the height of ϕ as a scattering length.

Band states: We have seen that a purely attractive potential (or more generally one whose space integral is < 0) will always have at least one BS 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 r -space. The k -space form of the TISE is (in any dimension)

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

Let's consider a very extended state, such that all k' 's 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

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

* S. Adhikari, Am. J. Phys. 54, 362 (1986); M. Raulo et al., PRB 41

It is debatable whether N_n is called a Bessel function of the second kind. † Abramowitz & Stegun ch. 9. The function $N_n(x)$ is often denoted $Y_n(x)$.

bound-state ($E < 0$)

It is clear that, whatever d , this eqn has no solution if $V_0 > 0$. If

$V_0 < 0$, then everything depends on the DOS as k (or $E \rightarrow 0$). The num

and k becomes in d dimensions $C_d \int d\epsilon \epsilon^{(d-1)/2}$, where C_d is a

constant; in particular, $C_2 = (m/2\pi\hbar^2)$. Thus the TISE reads

$$1 = |V_0| C_d \int_{-E}^{\epsilon_c} d\epsilon \frac{\epsilon^{(d-1)/2}}{\epsilon - E} \quad (V_0 < 0)$$

It is clear that this eqn always has a solution for $d=1$; for $d=3$ it

may or may not depending on the high-energy cut-off ϵ_c (which must be

determined e.g. by the dispersion of $V_{k=0}$ from the constant value V_0). For

$d=2$ a solution always exists, but the binding energy is exponential

small for $V_0 \rightarrow 0$:

$$E \approx \epsilon_c \exp - 1/(mV_0/2\pi\hbar^2)$$

(Cf. the solution of the Cooper problem in superconductivity theory which

is formally identical to a simple 2D Schrödinger problem since the relevant

DOS is similarly a constant)