

Для частицы массы m_0 в 1dPW с бесконечно высокими стенками при $x = 0$ и $x = L = 101\text{Å}$ построить аналитическим и численным $N = 100$ методами распределение плотности вероятности для $n = 1$ и $n = 25$.

```
clc, clear, close all
datetime('now')
```

```
ans = datetime
      17-May-2023 20:03:32
```

```
addpath('C:\Users\emill\Desktop\IORN\L07');
load('constance.mat', 'hbar', 'm0', 'J2eV');

L = 101 * 1e-10;
N = 100;
n_1 = 1;
n_2 = 25;
x = linspace(1e-10, L, N);
```

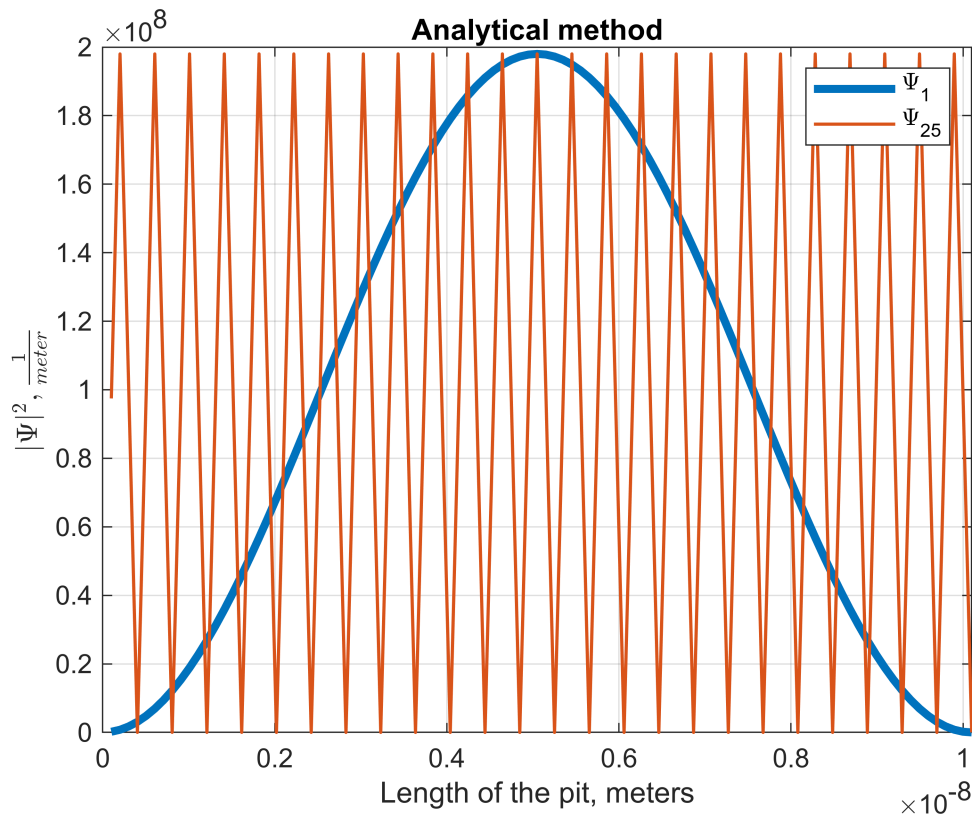
Analytical method

```
Psi_1_an = sqrt(2 / L) * sin(pi * n_1 * x ./ L);
Psi_2_an = sqrt(2 / L) * sin(pi * n_2 * x ./ L);

plot(x, abs(Psi_1_an) .^2, 'LineWidth', 3);
hold on;
plot(x, abs(Psi_2_an) .^2, 'LineWidth', 1.2);

xlabel("Length of the pit, meters");
ylabel("$|\Psi|^2, \{1\over meter}\$", 'Interpreter','latex');
legend("\Psi_{1}", "\Psi_{25}");
title('Analytical method');
grid on;
xlim([0, L]);

hold off;
```



Numerical method

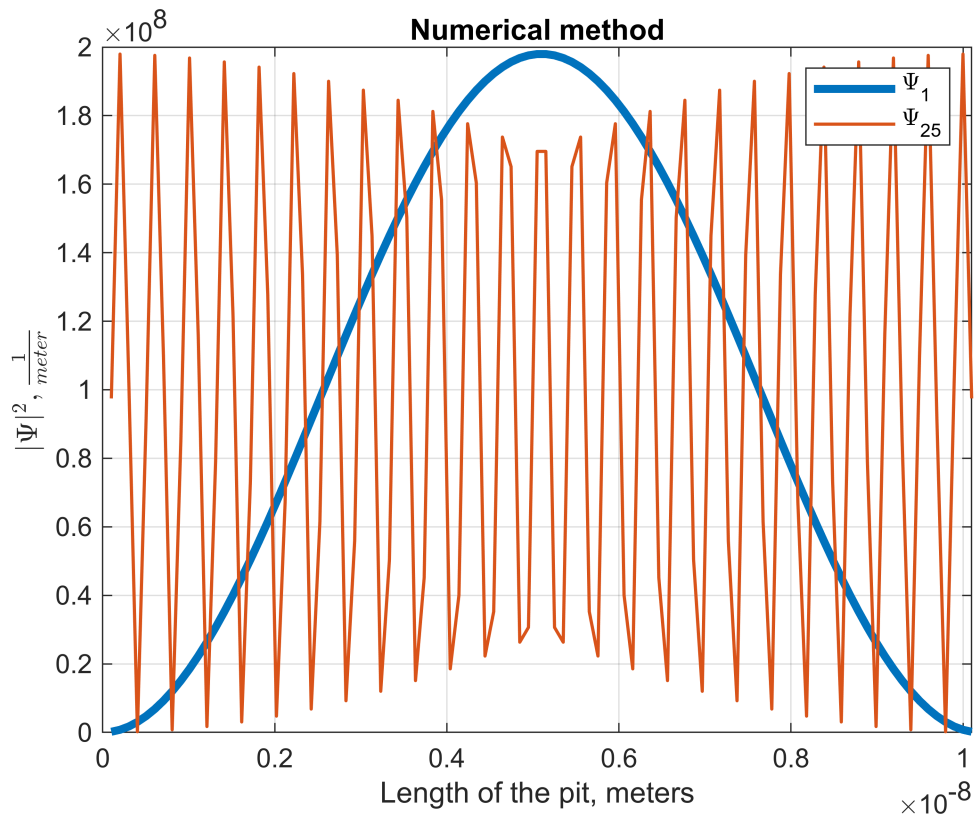
```
t = hbar ^ 2 / ((L / (N + 1)) ^ 2 * 2 * m0);
v_1 = 2 * t * ones(1, N);
v_2 = -t * ones(1, N - 1);
H = diag(v_1) + diag(v_2, 1) + diag(v_2, -1);
[V, D] = eig(H);

Psi_1_num = V(:, 1)';
Psi_2_num = V(:, 25)';

plot(x, abs(Psi_1_num) .^2 / (L / (N + 1)), 'LineWidth', 3);
hold on;
plot(x, abs(Psi_2_num) .^2 / (L / (N + 1)), 'LineWidth', 1.2);

xlabel("Length of the pit, meters");
ylabel("$|\Psi|^2, \frac{1}{\text{meter}}$", 'Interpreter', 'latex');
legend("\Psi_{1}", "\Psi_{25}");
title('Numerical method');
grid on;
xlim([0, L]);

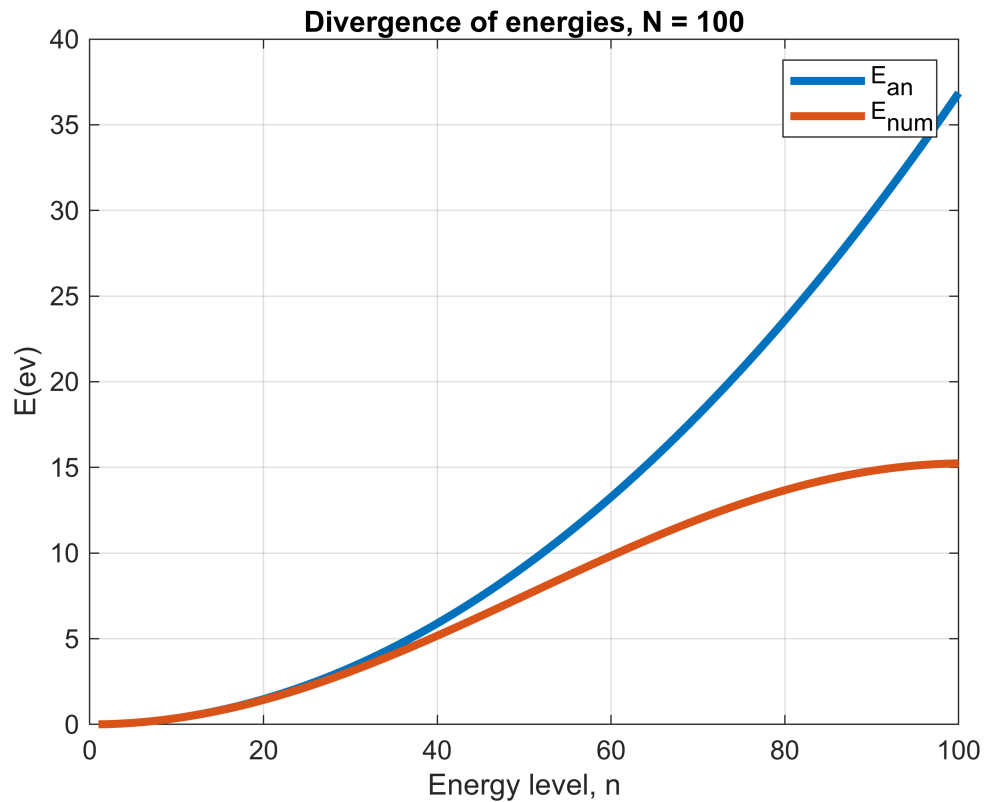
hold off;
```



Сравнение энергий

```
n = linspace(1, 100, N);
E_an = t * (pi * L / (N + 1) * n ./ L) .^ 2 * J2eV;
E_num = 2 * t * (1 - cos(pi * L / (N + 1) * n ./ L)) * J2eV;
plot(n, E_an, 'LineWidth', 3);
hold on;
plot(n, E_num, 'LineWidth', 3);

xlabel('Energy level, n');
ylabel('E(ev)');
legend('E_{an}', 'E_{num}');
title('Divergence of energies, N = 100');
xlim([0, 100]);
grid on;
hold off;
```



Подбор шага

```

k = n * pi / L;
E_1 = cos(k * L / (N + 1));
E_2 = 1 - k .^2 * (L / (N + 1)) ^ 2 / 2;

for i = 1 : numel(k)
    while(abs(E_1(i) - E_2(i)) > 1e-9)
        N = N + 1;
        n = linspace(1, 100, N);
        k = n * pi / L;
        E_1 = cos(k * L / (N + 1));
        E_2 = 1 - k .^2 * (L / (N + 1)) ^ 2 / 2;
    end
end

t = hbar ^ 2 / ((L / (N + 1)) ^ 2 * 2 * m0);
E_an = t * (pi * L / (N + 1) * n ./ L) .^ 2 * J2eV;
E_num = 2 * t * (1 - cos(pi * L / (N + 1) * n ./ L)) * J2eV;

plot(n, E_an, 'LineWidth', 7);
hold on;
plot(n, E_num, 'LineWidth', 3, 'LineStyle', '--');

xlabel('Energy level, n');
ylabel('E(ev)');

```

```

legend('E_{an}', 'E_{num}');
title(strjoin({'Divergence of energies, N = ', num2str(N)}));
xlim([0, 100]);
grid on;
hold off;

```

