HW 8-1 pb 4

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INFINITE SQUARE WELL VARIATIONAL CALCULATION
Potential: V = 0 for -a ¡ x ¡ a, V = $\infty elsewhere$
$Boundaryconditions : \psi(\pm a) = 0$
PART (a): TRAPEZOIDAL TRIAL FUNCTION
Trial function:
$\psi(x) = a - |x| forb \leq |x| \leq a(slopedregions)$
$\psi(x) = a - bfor|x| \leq b(flatregion)$
Case (i): b = 0 (Triangular function)
Normalization integral:
$N = \int_{-a}^{a}(a - |x|)^2 dx$
$Bysymmetry : N = 2\int_0^a (a - x)^2 dx$
$Expanding : \int_0^a (a^2 - 2ax + x^2)dx$
$= [a^2 x - ax^2 + x^3/3]_0^a$
$= a^3 - a^3 + a^3/3$
$= a^3/3$
A = $1/\sqrt{N} =$
Kinetic energy calculation:
$d\psi/dx = -Afor0 < x < a$
$d\psi/dx = +Afor - a < x < 0$
$< T >= (\hbar^2/2m)\int_{-a}^{a} |d\psi/dx|^2 dx$
$= (\hbar^2/2m) \times 2\int_0^a A^2 dx$
$= (\hbar^2/2m) \times 2A^2 a$
$= (\hbar^2/2m) \times$
$< E >= (\hbar^2/2m) \times /a^2$
$ANSWER(Casei) :< E >= [formula]\hbar^2/(2ma^2)$
Case (ii): Optimize parameter b
Normalization integral:
$N = \int_{-a}^{a} \psi^2 dx$
$= \int_{-a}^{-b}(a - |x|)^2 dx + \int_{-b}^{b}(a - b)^2 dx + \int_b^a (a - |x|)^2 dx$
By symmetry of outer regions:
$= 2\int_b^a (a - x)^2 dx + (a - b)^2(2b)$
$= 2[(a - x)^3/(-3)]_b^a + 2b(a - b)^2$
$= 2(a - b)^3/3 + 2b(a - b)^2$
N(b) =

Kinetic energy calculation:
$d\psi/dx = 0 for |x| < b (flat region contributes nothing)$
$d\psi/dx = -1 for b < x < a$
$d\psi/dx = +1 for - a < x < -b$
$< T >= (\hbar^2/2m) \times 2 \int_b^a (1/N) dx$
$= (\hbar^2/2m) \times 2(a-b)/N$
$= (\hbar^2/2m)\times$
Optimization:
$d < E > /db = (\hbar^2/2m)\times$
Since d¡E¿/db ¡ 0 for 0 ¡ b ¡ a, the energy decreases monotonically.
Therefore, the minimum occurs at b = 0 (triangular function).
ANSWER (Case ii): Optimal value b = 0 (triangular function gives minimum)
PART (b): PARABOLIC TRIAL FUNCTION
$Trial function : \psi(x) = A(x-a)(x+a) = A(x^2 - a^2)$
Normalization integral:
$N = \int_{-a}^a (x^2 - a^2)^2 dx$
$= \int_{-a}^a (x^4 - 2a^2x^2 + a^4) dx$
By symmetry (all terms are even):
$= 2\int_0^a (x^4 - 2a^2x^2 + a^4) dx$
$= 2[x^5/5 - 2a^2x^3/3 + a^4x]_0^a$
$= 2(a^5/5 - 2a^5/3 + a^5)$
$= 2a^5(1/5 - 2/3 + 1)$
$= 2a^5(3/15 - 10/15 + 15/15)$
$= 2a^5(8/15)$
$Derivative : d\psi/dx = 2Ax$
Kinetic energy calculation:
$< T >= (\hbar^2/2m) \int_{-a}^a |d\psi/dx|^2 dx$
$= (\hbar^2/2m) \int_{-a}^a (2Ax)^2 dx$
$= (\hbar^2/2m) \times 4A^2 \int_{-a}^a x^2 dx$
By symmetry:
$= (\hbar^2/2m) \times 4A^2 \times 2 \int_0^a x^2 dx$
$= (\hbar^2/2m) \times 8A^2 [x^3/3]_0^a$
$= (\hbar^2/2m) \times 8A^2a^3/3$
$= (\hbar^2/2m)\times$
$< E >= (\hbar^2/2m) \times /a^2$
$ANSWER(Part b) :< E >= [formula]\hbar^2/(2ma^2)$
PART (c): QUARTIC TRIAL FUNCTION
$Trial function : \psi(x) = (a^2 - x^2)(\alpha x^2 + \beta)$
$Variational parameter : r = \alpha/\beta$
$Expanding : \psi(x) = (a^2 - x^2)(\alpha x^2 + \beta) = \alpha a^2 x^2 + \beta a^2 - \alpha x^4 - \beta x^2$
Normalization integral:
$N = \int_{-a}^a [(a^2 - x^2)(\alpha x^2 + \beta)]^2 dx$
$= \int_{-a}^a [(\alpha a^2x^2 + \beta a^2)^2 - 2(\alpha a^2x^2 + \beta a^2)(\alpha x^4 + \beta x^2) + (\alpha x^4 + \beta x^2)^2] dx$
(All terms are even functions, so we integrate over symmetric limits)

Derivative calculation:
$d\psi/dx = d/dx[(a^2 - x^2)(\alpha x^2 + \beta)]$
$Using product rule := (a^2 - x^2)(2\alpha x) + (\alpha x^2 + \beta)(-2x)$
$= 2\alpha x(a^2 - x^2) - 2x(\alpha x^2 + \beta)$
$= 2\alpha a^2 x - 2\alpha x^3 - 2\alpha x^3 - 2\beta x$
$= 2\alpha a^2 x - 4\alpha x^3 - 2\beta x$
$d\psi/dx =$
Kinetic energy integral:
$< T >= (\hbar^2/2m) \int_{-a}^{a} |d\psi/dx|^2 dx/N$
$= (\hbar^2/2m) \int_{-a}^{a} (2\alpha a^2 x - 4\alpha x^3 - 2\beta x)^2 dx/N$
(Even function integrated over symmetric limits)
Numerator =
$< T >= (\hbar^2/2m)\times$
$Energy as function of r = \alpha/\beta :$
$< E > (r) = (\hbar^2/2m)\times$
Variational condition d¡E¿/dr = 0:
$d < E > /dr = (\hbar^2/2m)\times$
Solutions for optimal r:
$r_1 =$
$r_2 =$
Energy values:
$At r_1 :< E >= (\hbar^2/2m) \times /a^2$
$At r_2 :< E >= (\hbar^2/2m) \times /a^2$
$Selecting r_2 (minimum energy)$
Optimal parameters:
$r_{opt} =$
$< E >= (\hbar^2/2m) \times /a^2$

ANSWER (Part c):
Optimal r = formula]
$< E >= formula]\hbar^2/(2ma^2)$

PART (d): COMPARISON WITH EXACT RESULT
Exact ground state:
$\psi_0(x) = (1/\sqrt{a}) cos(\pi x/(2a))$
$E_0 = \pi^2\hbar^2/(8ma^2) = (\hbar^2/2m)\times$
Summary of Variational Estimates
$Method < E > in units of (\hbar^2/2m)/a^2$
Exact
Triangular
Parabolic
Quartic (optimized)
$Verification : All variational estimates satisfy < E >\geq E_0$
$Triangular :\geq \checkmark$
$Parabolic :\geq \checkmark$
$Quartic :\geq \checkmark$

ANSWER (Part d):
$All variational estimates satisfy < E >\geq E$ 0   The quartic trial function gives the best approximation.

Mean-Square Deviations

$Formula : \Delta^2 = \int |\psi_0 - \psi_t|^2 dx = 2(1 - \int \psi_0\psi_t dx) for normalized functions$

Parabolic function:

$Overlap : \int_{-a}^{a} \psi_0\psi_t dx =$

$Mean - square deviation : \Delta^2 =$

$Interpretation : Smaller \Delta^2 indicates better approximation to exact ground state.$

PART (e): NODES OF OPTIMAL QUARTIC AND INTERPRETATION

$Optimized quartic : \psi(x) = A(a^2 - x^2)(\alpha x^2 + \beta) with r = \alpha/\beta =$

Nodes occur at:

$(1) Boundary : x = \pm a (required by boundary conditions)$

$(2) Interior : where \alpha x^2 + \beta = 0, i.e., x^2 = -\beta/\alpha = -1/r$

$Interior node condition : x^2 = -1/r =$

$Real interior nodes exist at x^2 = Location : INSIDE the well (|x| < a) Location : OUTSIDE the well (|x| > a) No real interior nodes (x^2 < 0)$

Interpretation of Stationary Energy Value

The variational method minimizes ¡E¿ within the family of quartic trial functions.

At the stationary point (d¡E¿/dr = 0):

$\bullet The energy is minimized with respect to the parameter r$

$\bullet This provides an upper bound :< E >\geq E_0 (variational theorem)$

$\bullet The optimal function best approximates the true ground state within this family$

Physical significance:

$\bullet The optimization balances kinetic energy (prefers smoothness) with boundary conditions (requires \psi(\pm a) = 0)$

$\bullet The true ground state cos(\pi x/2a) has NO interior nodes$

$\bullet Our quartic approximation may have nodes depending on the parameter space$

$\bullet The stationary condition d < E > /dr = 0 is the variational analog of the Schrödinger equation, ensuring the functional derivative vanishes$

ANSWER (Part e):
$The stationary energy represents the best approximation to E$ 0 $within the chosen family, guaranteed to be \geq E$ 0.